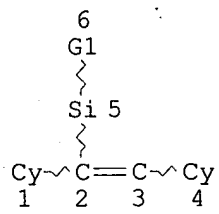
Hui, S.
09/590447

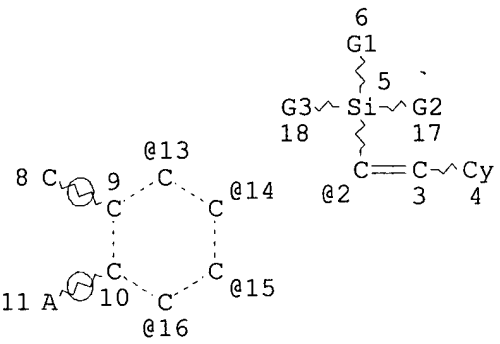
FILE 'REGISTRY' ENTERED AT 11:49:17 ON 23 MAY 2002
L1 STR



VAR G1=AK/CB
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 1
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
L3 67 SEA FILE=REGISTRY SSS FUL L1
L5 STR



VAR G1=AK/CB
VAR G2=AK/CB
VAR G3=AK/CB
VPA 2-13/14/15/16 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L6 26 SEA FILE=REGISTRY SUB=L3 SSS FUL L5

100.0% PROCESSED 34 ITERATIONS 26 ANSWERS
SEARCH TIME: 00.00.01

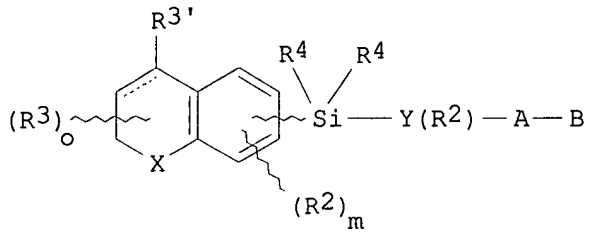
(FILE 'CAPLUS' ENTERED AT 11:50:25 ON 23 MAY 2002)
L7 3 S L6 OR L6/D

Date, not good

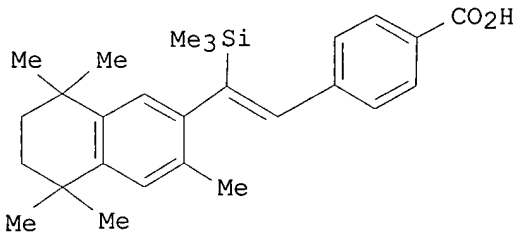
L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:900648 CAPLUS
DOCUMENT NUMBER: 134:42260
TITLE: Organosilyl compounds having nuclear hormone receptor modulating activity
INVENTOR(S): Beard, Richard L.; Garst, Michael; Chandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000077011	A1	20001221	WO 2000-US15972	20000609
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1185539	A1	20020313	EP 2000-941321	20000609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000011741	A	20020319	BR 2000-11741	20000609

PRIORITY APPLN. INFO.: US 1999-138731P P 19990611
WO 2000-US15972 W 20000609
OTHER SOURCE(S): MARPAT 134:42260
GI



I



II

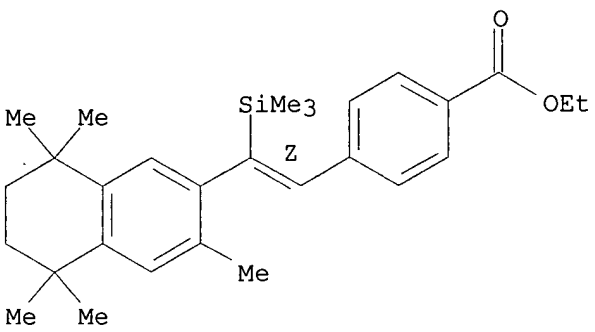
AB The prepn. of silicon-contg. org. compds., I (X = O, S, NR', R' = C1-6 alkyl; R2 = H, C1-6 alkyl, F, Cl, Br, I, CF3, OH, SH, C1-12 alkoxy, alkylthio, etc.; R3 = H, C1-6 alkyl, F; m = 0-3; o = 0-4; R3' = H, C1-6 alkyl, F, heteroaryl with 1-3 hetero atoms, etc.; R4 = C1-8 alkyl, Ph, etc.; Y = Ph, naphthyl, heteroaryl, etc.; A = (CH2)q, q = C3-6 alkyl, C3-6 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl, etc.; B = H, CO2H, NO2, P(O)(OH)2, etc.), useful as modulators of mammalian nuclear hormone receptors, particularly the retinoid receptors and the farnesoid receptors, is described. Thus, silylation of 4-BrC6H4CH2OH with Ph2(t-Bu)SiCl in CH2Cl2 in the presence of Et3N gave 4-BrC6H4CH2OSiPh2Bu-t which on coupling with Me3SiC.tplbond.CH gave 4-Me3SiC.tplbond.CC6H4CH2OSiPh2Bu-t. Borane mediated coupling of 4-Me3SiC.tplbond.CC6H4CH2OSiPh2Bu-t with 2-bromo-3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalene followed by MnO2 oxidn. and hydrolysis gave title compd. II.

IT **312738-41-3P 312738-52-6P 312738-57-1P 312738-65-1P 312738-69-5P 312738-79-7P 312738-82-2P 312738-86-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

RN 312738-41-3 CAPLUS

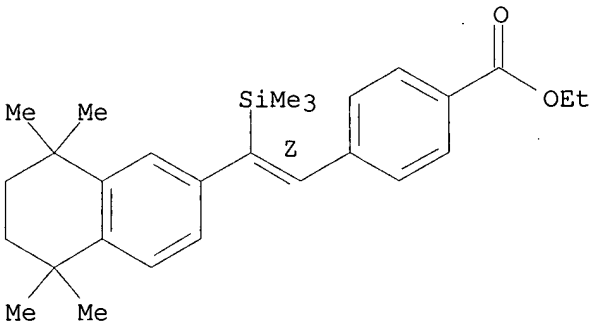
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



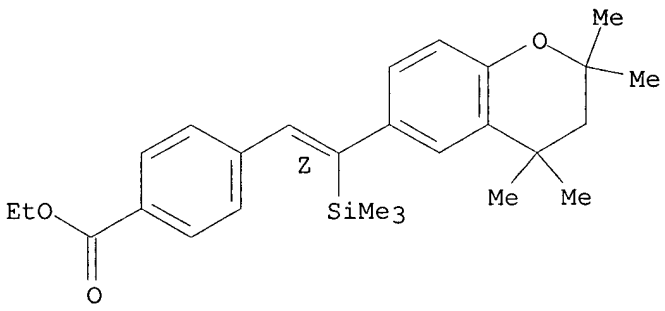
RN 312738-52-6 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 312738-57-1 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(3,4-dihydro-2,2,4,4-tetramethyl-2H-1-benzopyran-6-yl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

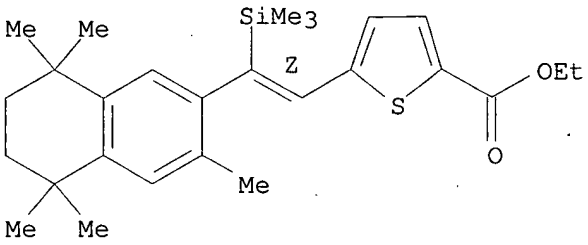
Double bond geometry as shown.



RN 312738-65-1 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-

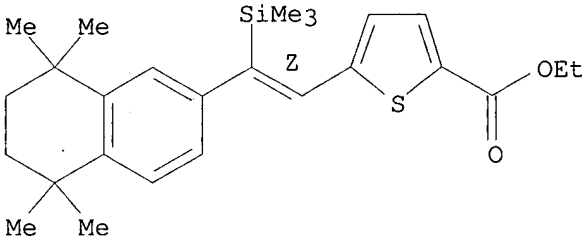
pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



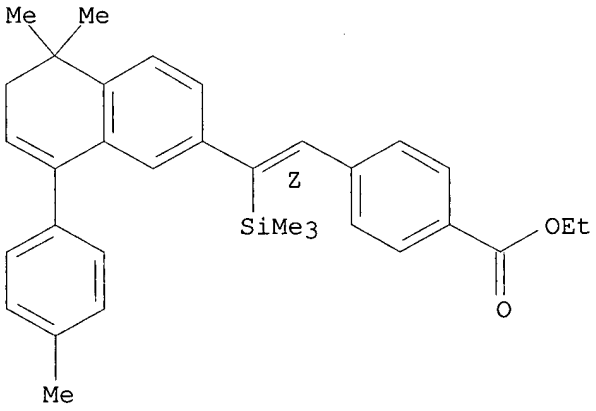
RN 312738-69-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



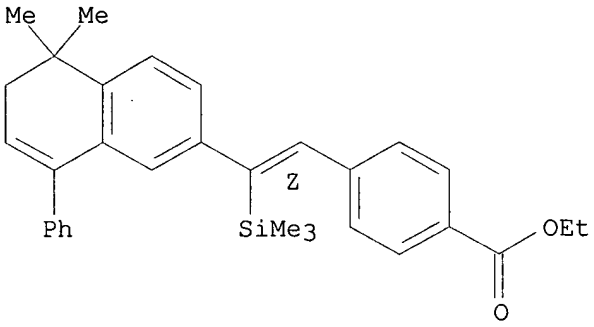
RN 312738-79-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



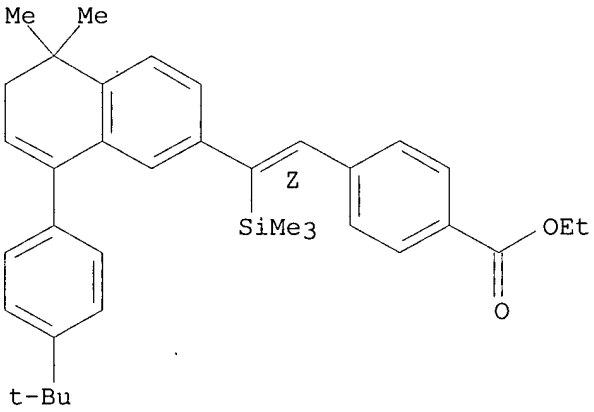
RN 312738-82-2 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



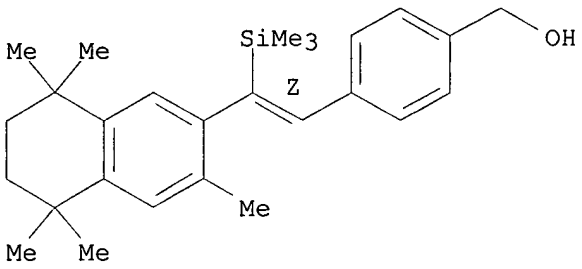
RN 312738-86-6 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



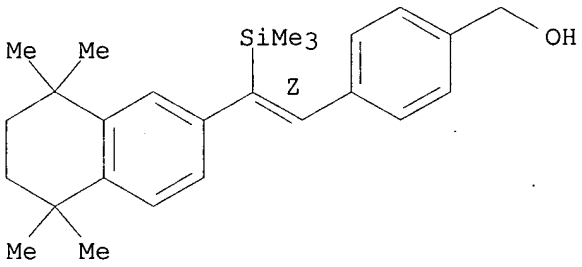
IT **312738-36-6P 312738-49-1P 312738-64-0P**
312738-68-4P 312738-77-5P 312738-81-1P
312738-85-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
RN 312738-36-6 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



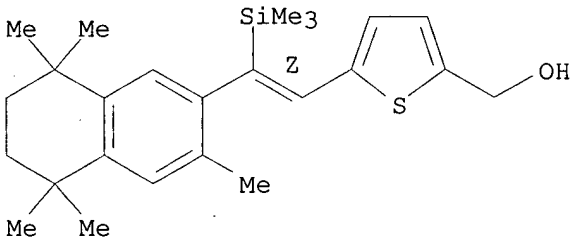
RN 312738-49-1 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



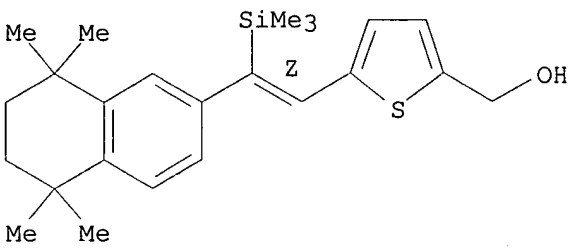
RN 312738-64-0 CAPLUS
CN 2-Thiophenemethanol, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



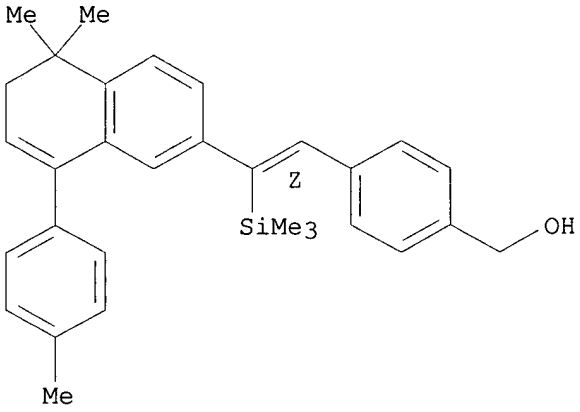
RN 312738-68-4 CAPLUS
CN 2-Thiophenemethanol, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



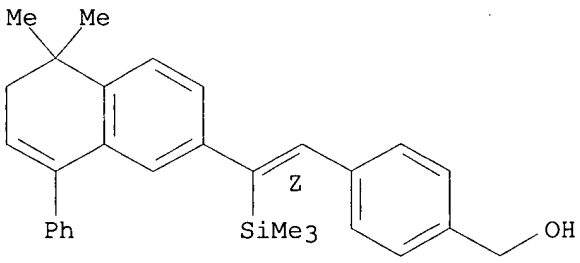
RN 312738-77-5 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



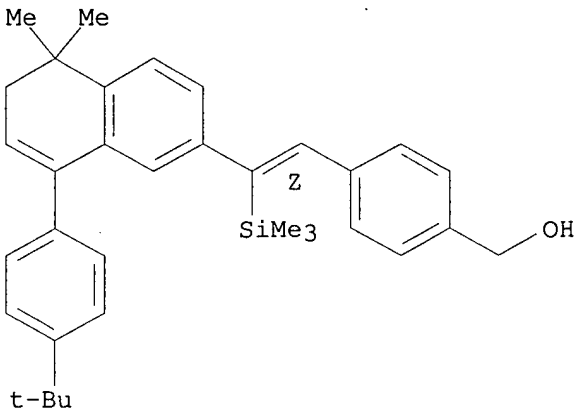
RN 312738-81-1 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



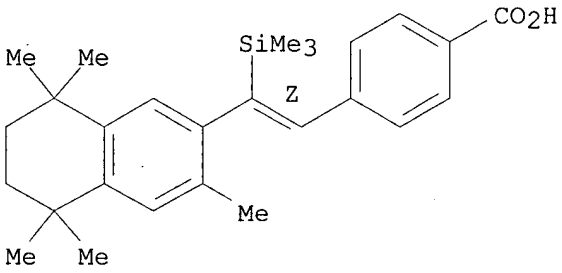
RN 312738-85-5 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



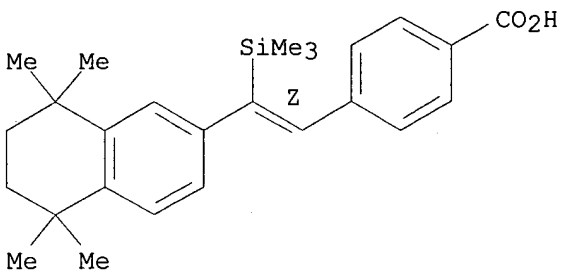
IT **312738-45-7P 312738-55-9P 312738-58-2P**
312738-67-3P 312738-70-8P 312738-80-0P
312738-84-4P 312738-87-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of organosilyl compds. having nuclear hormone receptor modulating activity)
RN 312738-45-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



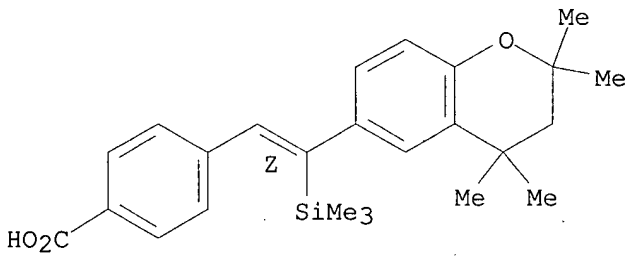
RN 312738-55-9 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



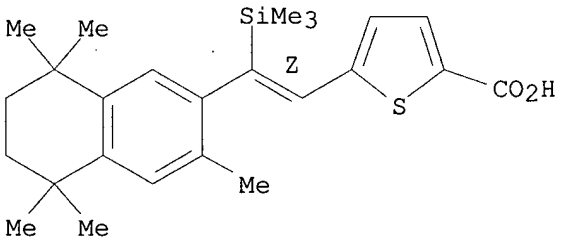
RN 312738-58-2 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(3,4-dihydro-2,2,4,4-tetramethyl-2H-1-benzopyran-6-yl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



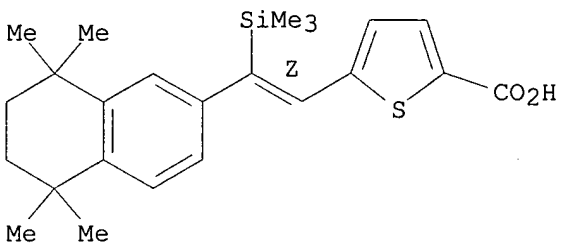
RN 312738-67-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



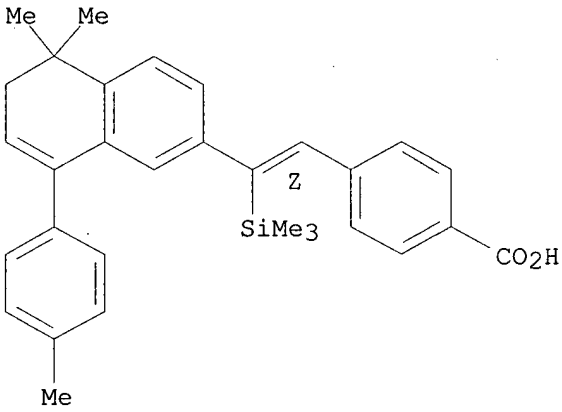
RN 312738-70-8 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



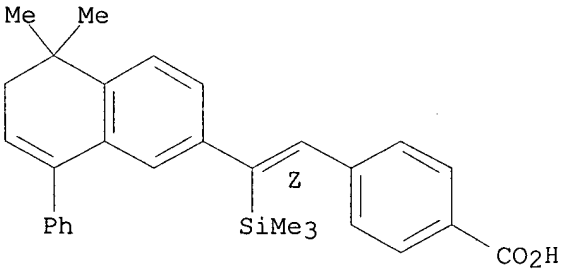
RN 312738-80-0 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



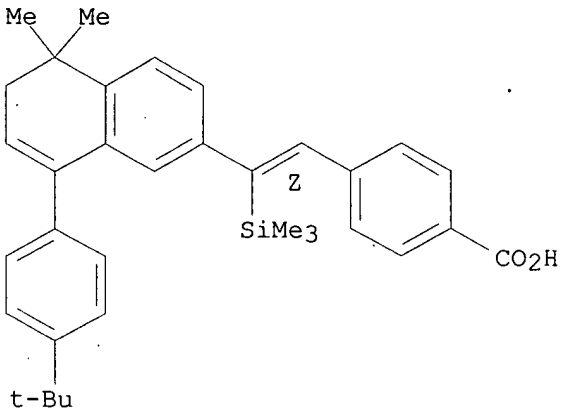
RN 312738-84-4 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 312738-87-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:900465 CAPLUS
DOCUMENT NUMBER: 134:37038
TITLE: Methods for modulating FXR receptor activity
INVENTOR(S): Forman, Barry M.; Beard, Richard L.; Gyhandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

Bad date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000076523	A1	20001221	WO 2000-US15912	20000609
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1185277	A1	20020313	EP 2000-941312	20000609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: US 1999-138731P P 19990611
WO 2000-US15912 W 20000609
OTHER SOURCE(S): MARPAT 134:37038

AB Methods for modulating the activity of the mammalian FXR (farnesoid X-activated receptor). The methods include methods of treating a hyper- or hypocholesterolemic mammal comprising contacting the

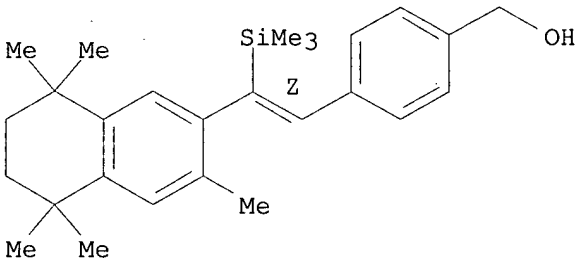
mammal with synthetic compds. having FXR receptor activity.

IT **312738-36-6P 312738-41-3P 312738-49-1P**
312738-52-6P 312738-57-1P 312738-64-0P
312738-65-1P 312738-68-4P 312738-69-5P
312738-77-5P 312738-79-7P 312738-81-1P
312738-82-2P 312738-85-5P 312738-86-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

RN 312738-36-6 CAPLUS

CN Benzenemethanol, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

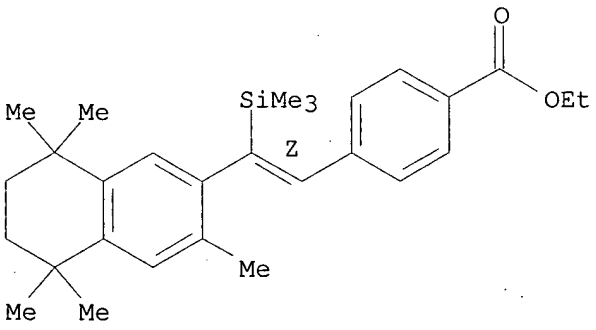
Double bond geometry as shown.



RN 312738-41-3 CAPLUS

CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

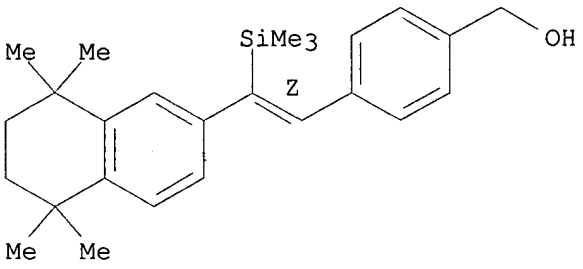
Double bond geometry as shown.



RN 312738-49-1 CAPLUS

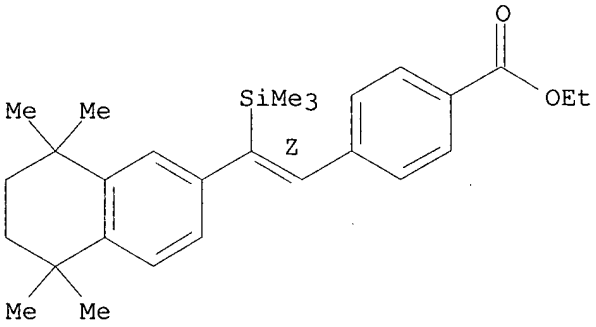
CN Benzenemethanol, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



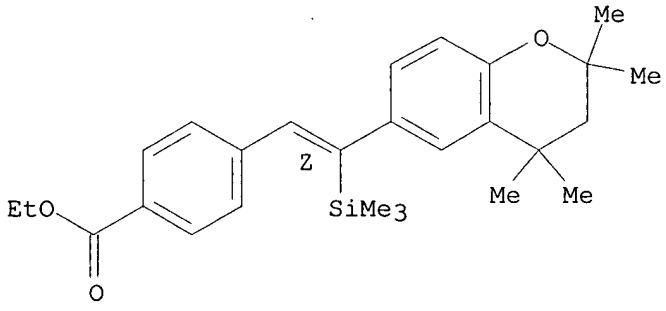
RN 312738-52-6 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



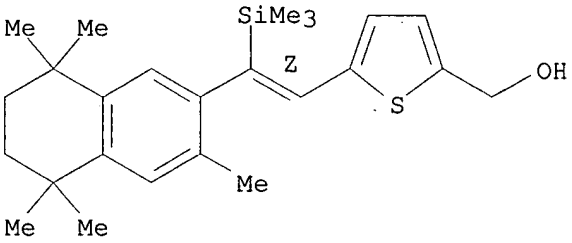
RN 312738-57-1 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(3,4-dihydro-2,2,4,4-tetramethyl-2H-1-benzopyran-6-yl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



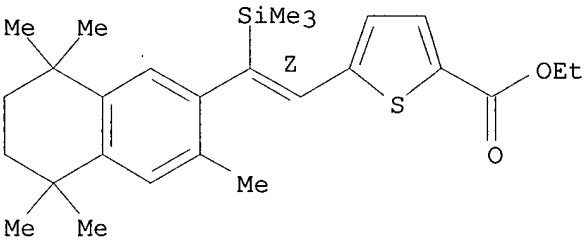
RN 312738-64-0 CAPLUS
CN 2-Thiophenemethanol, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



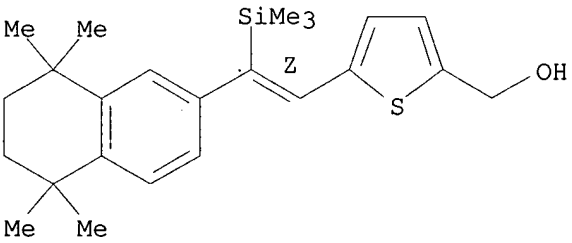
RN 312738-65-1 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



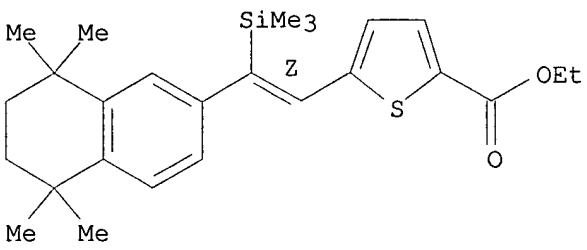
RN 312738-68-4 CAPLUS
CN 2-Thiophenemethanol, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



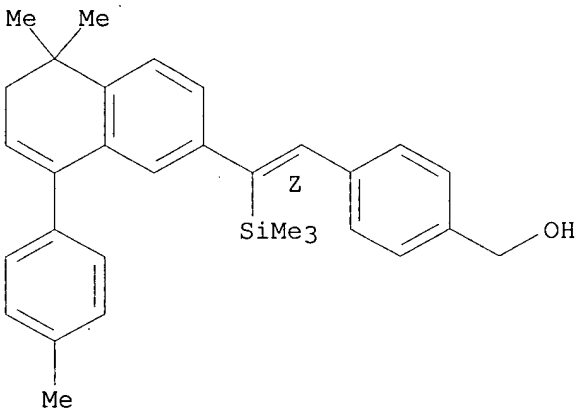
RN 312738-69-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



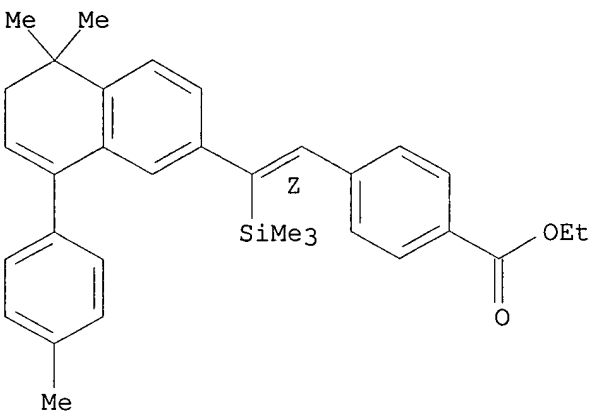
RN 312738-77-5 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



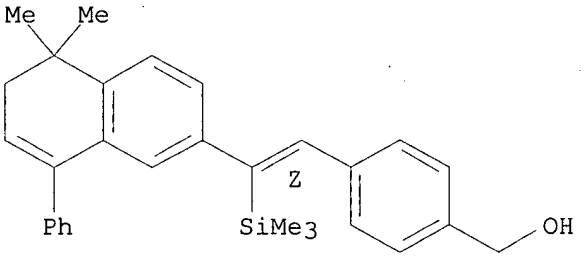
RN 312738-79-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



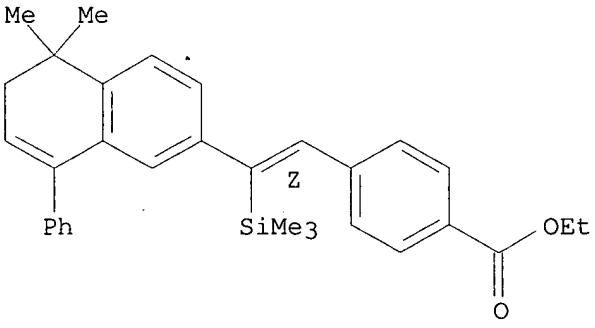
RN 312738-81-1 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 312738-82-2 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

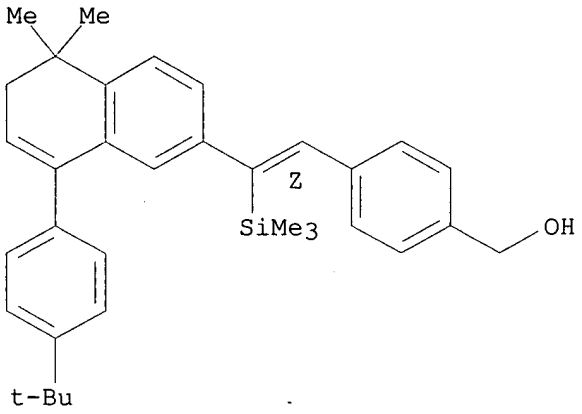
Double bond geometry as shown.



RN 312738-85-5 CAPLUS
CN Benzenemethanol, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-

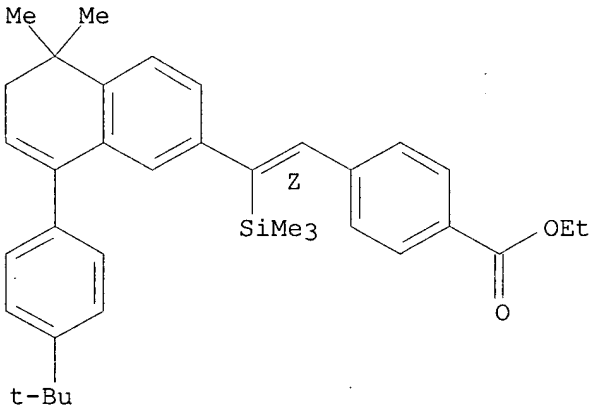
dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 312738-86-6 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

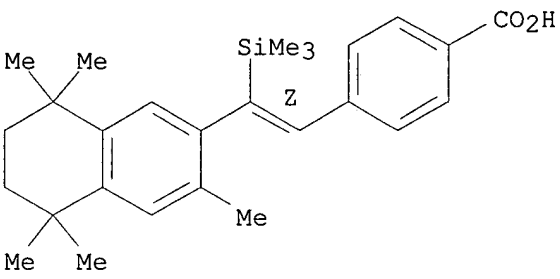
Double bond geometry as shown.



IT **312738-45-7P 312738-55-9P 312738-58-2P**
312738-67-3P 312738-70-8P 312738-80-0P
312738-84-4P 312738-87-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)
RN 312738-45-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-

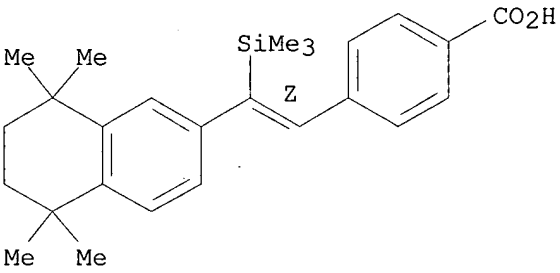
naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



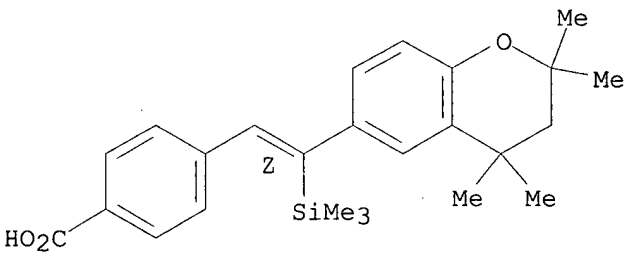
RN 312738-55-9 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



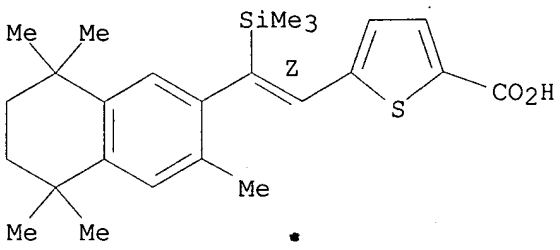
RN 312738-58-2 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(3,4-dihydro-2,2,4,4-tetramethyl-2H-1-benzopyran-6-yl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



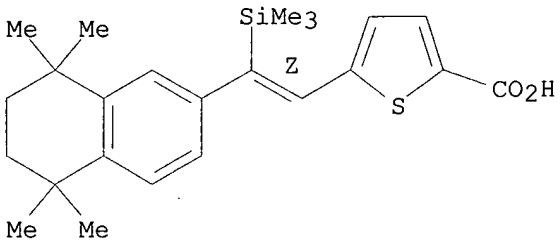
RN 312738-67-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



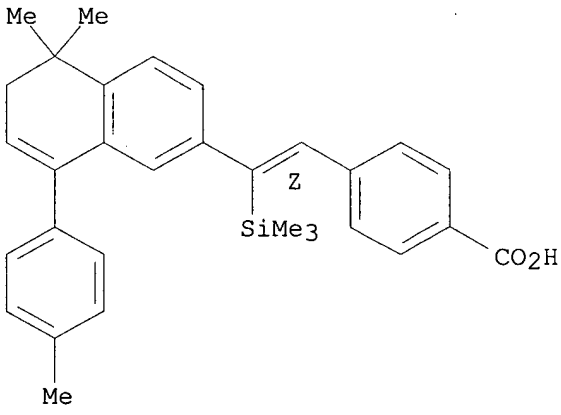
RN 312738-70-8 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



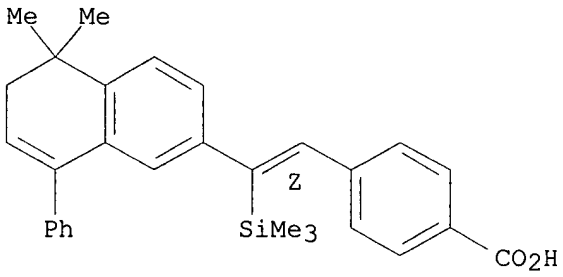
RN 312738-80-0 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[5,6-dihydro-5,5-dimethyl-8-(4-methylphenyl)-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



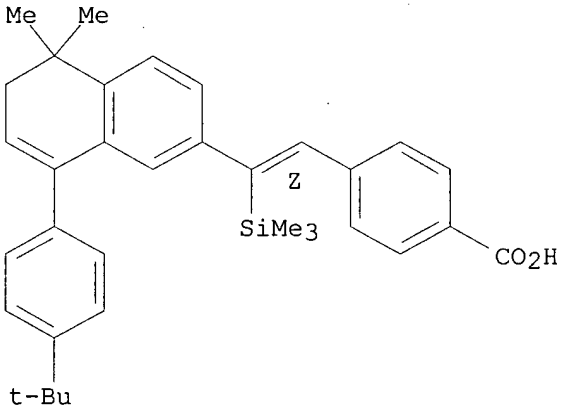
RN 312738-84-4 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-(5,6-dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



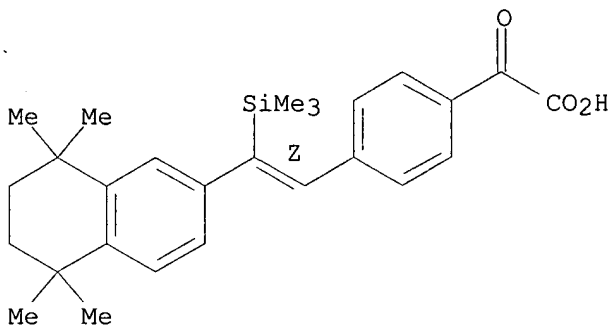
RN 312738-87-7 CAPLUS
CN Benzoic acid, 4-[(1Z)-2-[8-[4-(1,1-dimethylethyl)phenyl]-5,6-dihydro-5,5-dimethyl-2-naphthalenyl]-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **313268-94-9**, AGN 10
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)
RN 313268-94-9 CAPLUS
CN Benzeneacetic acid, .alpha.-oxo-4-[(1Z)-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-2-(trimethylsilyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



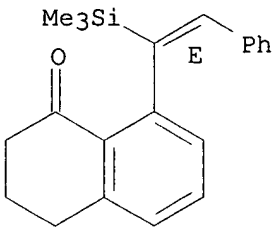
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:455381 CAPLUS
DOCUMENT NUMBER: 125:114330
TITLE: Preparation of highly unsaturated carbonyl compounds by addition reaction of .alpha.,.beta.-unsaturated carbonyl compounds with acetylenes
INVENTOR(S): Murai, Shinji; Chatani, Naoto; Kakiuchi, Fumitoshi
PATENT ASSIGNEE(S): Shingijutsu Kaihatsu Jigyodan, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08127551	A2	19960521	JP 1994-266565	19941031

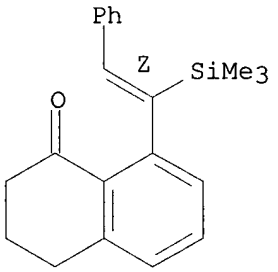
OTHER SOURCE(S): CASREACT 125:114330; MARPAT 125:114330
AB Compds. having COC:CC:CH group are prepd. by treatment of compds. having COC:CH group with acetylenic C.tplbond.C compds. in the presence of transition metal catalysts. .alpha.-Tetralone was refluxed with PrC.tplbond.CPr and RuH2(CO)(PPh3)3 in MePh for 4 h to give 72% 8-(4-octen-5-yl)-.alpha.-tetralone with E/Z = 16/1 ratio.
IT **179039-10-2P 179039-11-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of highly unsatd. carbonyl compds. from .alpha.,.beta.-unsatd. carbonyl compds. with acetylenes)
RN 179039-10-2 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-8-[2-phenyl-1-(trimethylsilyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 179039-11-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-8-[2-phenyl-1-(trimethylsilyl)ethenyl]-, (Z)- (9CI) (CA INDEX NAME)

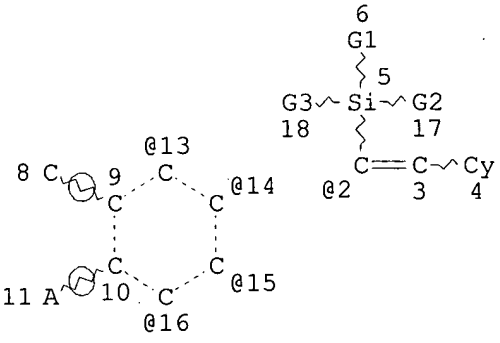
Double bond geometry as shown.



FILE 'CAOLD' ENTERED AT 11:52:03 ON 23 MAY 2002
L8 0 S L6

FILE 'USPATFULL' ENTERED AT 11:52:09 ON 23 MAY 2002
L9 0 S L6

(FILE 'MARPAT' ENTERED AT 11:52:21 ON 23 MAY 2002)
L5 STR



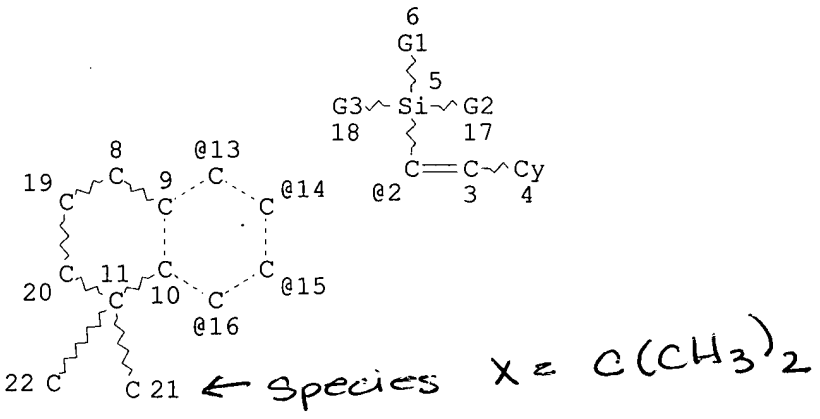
VAR G1=AK/CB
VAR G2=AK/CB
VAR G3=AK/CB
VPA 2-13/14/15/16 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
MLEVEL IS CLASS ON RING NODES AND RING GROUPS
MLEVEL IS CLASS ON CHAIN NODES AND CHAIN GROUPS
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L11 136 SEA FILE=MARPAT SSS FUL L5 (MODIFIED ATTRIBUTES)
L12 STR



← species X = $C(CH_3)_2$

VAR G1=AK/CB
VAR G2=AK/CB
VAR G3=AK/CB
VPA 2-13/14/15/16 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
MLEVEL IS CLASS ON RING NODES AND RING GROUPS
MLEVEL IS CLASS ON CHAIN NODES AND CHAIN GROUPS
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L13 18 SEA FILE=MARPAT SUB=L11 SSS FUL L12 (MODIFIED ATTRIBUTES)

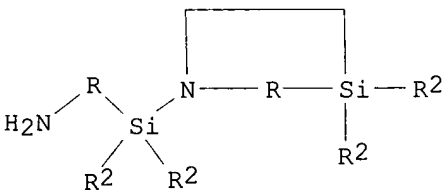
100.0% PROCESSED 134 ITERATIONS (1 INCOMPLETE) 18 ANSWERS
SEARCH TIME: 00.01.10

L13 ANSWER 1 OF 18 MARPAT COPYRIGHT 2002 ACS

(ALL HITs ARE ITERATION INCOMPLETES)
ACCESSION NUMBER: 136:102511 MARPAT
TITLE: Preparation of cyclic silazanes
INVENTOR(S): Schaefer, Oliver; Bauer, Andreas; Brader, Leonhard; Pachaly, Bernd; Frey, Volker
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie Gmbh, Germany
SOURCE: Ger., 6 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10049183	C1	20020117	DE 2000-10049183	20001005
EP 1195379	A1	20020410	EP 2001-117799	20010802
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2002042491	A1	20020411	US 2001-965902	20010927

PRIORITY APPLN. INFO.: DE 2000-10049183 20001005
OTHER SOURCE(S): CASREACT 136:102511
GI



I

AB The prepn. of title compds., I (R = divalent Si-C and Si-N bonded optionally cyano or halo-substituted C3-15 hydrocarbon, etc.; R1 = H, monovalent halo substituted Si-C bonded C1-15 hydrocarbon, etc.; R2 = H, monovalent halo or cyano substituted Si-C bonded C1-20 hydrocarbon, etc.), is described. Thus, ammonolysis of 3-chloropropyldimethylchlorosilane in a autoclave gave N-{(3-aminopropyl)dimethylsilyl}-2,2-dimethyl-1-aza-2-silacyclopentane which on hydrolysis with H2O/THF gave 95% bis(3-aminopropyl)tetramethyldisiloxane.

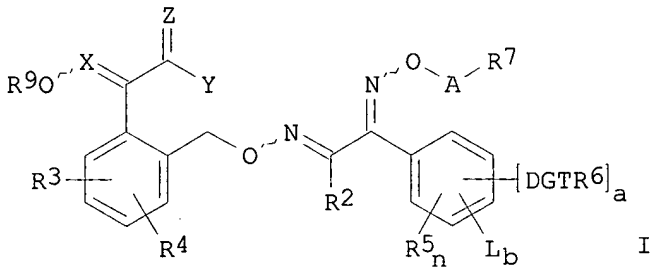
IC ICM C07F007-10
ICS C07F007-18
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35
ST cyclic silazane prepn hydrolysis; disiloxane aminopropyl prepn
IT Silazanes
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cyclic)
IT 10605-40-0, 3-Chloropropyldimethylchlorosilane 388613-96-5
RL: RCT (Reactant); RACT (Reactant or reagent)

(ammonolysis of)
IT 388606-32-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
IT 2469-55-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

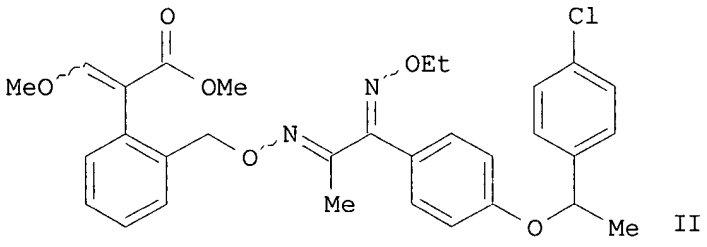
L13 ANSWER 2 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 135:344274 MARPAT
TITLE: Preparation of O-benzyl oxime ethers as pesticides
INVENTOR(S): Trah, Stephan; Szczepanski, Henry; Huter, Ottmar Franz; Hall, Roger Graham; Farooq, Saleem; Pascual, Alfons
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: U.S., 33 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6313344	B1	20011106	US 1998-85283	19980527

GI



I



II

AB The title compds. [I; either X = CH, N; Y = OR1; Z = O, or X = N; Y

= NHR8, Z = O, S, S(O); R1-R4 = H, C1-4 alkyl, etc.; R5 = halo, alkyl, haloalkyl, etc.; n = 0-4; R8 = H, C1-4 alkyl; R9 = Me, CH2F, CHF2; A = a direct bond, C(O), C(S), etc.; R7 = CN, OH, OC1-6 alkyl, etc.; D = O, S, S(O), S(O)2; G = C1-8 alkylene; TR6 = R6, C(O)R6; C.tplbond.CR6, etc.; R6 = alkyl, (un)substituted aryl, heteroaryl; L = UR18, P(O)vR11R12, etc.; v = 0-1; UR18 = C(O)C(O)R18, C(OH)C(OH)R18, etc.; a = 0-1; b = 0-1; R11, R12 = alkyl, haloalkyl, cycloalkyl; R18 = R6], useful in controlling pests, were prepd. Thus, treatment of 1-{4-[1-(4-chlorophenyl)ethoxy]phenyl}-1,2-propanedione-(ethyloxime)-2-oxime (prepn. given) with NaH in DMF followed by addn. of 2-(bromomethyl)-.alpha.-(methoxymethylene)phenylacetic acid Me ester in DMF afforded (E)-II which was more than 80% effective against Aphis craccivora and Diabrotica balteata.

IC ICM C07C327-00
NCL 564074000
CC 25-5 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
ST benzyl oxime ether prepn pesticide
IT Pesticides
(prepn. of O-benzyl oxime ethers as pesticides)
IT 216667-97-9P 216674-48-5P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of O-benzyl oxime ethers as pesticides)
IT 216667-88-8P 216668-04-1P 216668-11-0P 216668-21-2P
216668-29-0P 216668-36-9P 216668-44-9P 216668-52-9P
216668-58-5P 216668-64-3P 216668-70-1P 216668-77-8P
216668-85-8P 216668-92-7P 216668-99-4P 216669-06-6P
216669-12-4P 216669-19-1P 216669-24-8P 216669-33-9P
216669-39-5P 216669-46-4P 216669-52-2P 216669-59-9P
216669-65-7P 216669-70-4P 216669-76-0P 216669-85-1P
216669-93-1P 216670-01-8P 216670-09-6P 216670-15-4P
216670-25-6P 216670-32-5P 216670-39-2P 216670-51-8P
216670-59-6P 216670-67-6P 216670-76-7P 216670-86-9P
216670-97-2P 216671-09-9P 216671-18-0P 216671-27-1P
216671-37-3P 216671-49-7P 216671-57-7P 216671-68-0P
216671-76-0P 216671-84-0P 216671-95-3P 216672-04-7P
216672-13-8P 216672-25-2P 216672-34-3P 216672-42-3P
216672-52-5P 216672-66-1P 216672-77-4P 216672-87-6P
216673-00-6P 216673-08-4P 216673-17-5P 216673-26-6P
216673-35-7P 216673-46-0P 216673-57-3P 216673-68-6P
216673-75-5P 216673-83-5P 216673-89-1P 216673-95-9P
216674-01-0P 216674-07-6P 216674-15-6P 216674-21-4P
216674-28-1P 216674-35-0P 216674-42-9P 216674-52-1P
216674-57-6P 216674-60-1P 216674-62-3P 216674-65-6P
216674-69-0P 216674-73-6P 216674-80-5P 216674-82-7P
216674-83-8P 216674-85-0P 216674-87-2P 216674-88-3P
216674-90-7P 216674-91-8P 216674-94-1P 216674-96-3P
216674-98-5P 216674-99-6P 216675-02-4P 216675-03-5P
216675-05-7P 216675-09-1P 216675-10-4P 216675-11-5P
216675-13-7P 216675-15-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of O-benzyl oxime ethers as pesticides)
IT 106-47-8, 4-Chloroaniline, reactions 456-03-1, 4-Fluoropropiophenone 460-00-4, 4-Bromofluorobenzene 536-38-9 762-04-9, Diethyl phosphite 770-39-8, 1-(4-Hydroxyphenyl)propan-2-one 1719-57-9, (Chloromethyl)dimethylsilyl chloride 3391-10-4, 1-(4-Chlorophenyl)ethanol 4937-87-5 107048-59-9 115199-26-3 170732-31-7 187347-38-2 216675-57-9 216675-59-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of O-benzyl oxime ethers as pesticides)
IT 770-90-1P 69617-60-3P 152801-67-7P 216675-17-1P 216675-18-2P 216675-20-6P 216675-25-1P 216675-27-3P 216675-30-8P 216675-33-1P 216675-34-2P 216675-36-4P 216675-39-7P 216675-40-0P 216675-42-2P 216675-45-5P 216675-47-7P 216675-49-9P 216675-51-3P 216675-52-4P 216675-54-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of O-benzyl oxime ethers as pesticides)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 134:86630 MARPAT
TITLE: Production method of 1,4-dienes with high selectivity
INVENTOR(S): Sakai, Tatsuya
PATENT ASSIGNEE(S): JSR Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Bad date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001010982	A2	20010116	JP 1999-178946	19990624

AB 1,4-Dienes represented by the general formula CH2:CHCH2CH:CR1CHR2R3 are obtained by a reaction of ethylene with 1,3-diens represented by the general formula CH2:CHCR1:CR2R3 at 50-100.degree. under .gtoreq.3 MPa pressure for 3 min to 2 h in the presence of Fe compds. and organoaluminum compds. represented by the general formula R4nAlZn-3, where R1-3 = H, halogen, C1-20 hydrocarbyl, C1-20 halogenated hydrocarbyl, or alkylsilyl (excluding R1 = R2 = R3 = H), R4 = C1-20 monovalent hydrocarbyl, Z = H, alkoxyl, or halogen, and 0 < n .ltoreq. 3. Thus, 500 g isoprene was reacted with ethylene at 80.degree. for 2 h under 3 MPa pressure in the presence of 1.5 mmol triethylaluminum and 0.5 mmol iron(III) acetylacetonate to give 50:50 5-methyl-1,4-hexadiene/4-methyl-1,4-hexadiene with yield 85%.
IC ICM C07C002-40
ICS B01J031-20; C07C011-12; C07C015-44; C07B061-00
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 23
ST diene prepn isoprene ethylene
IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(1,3-; prepn. of 1,4-dienes with high selectivity from 1,3-diens and ethylene)

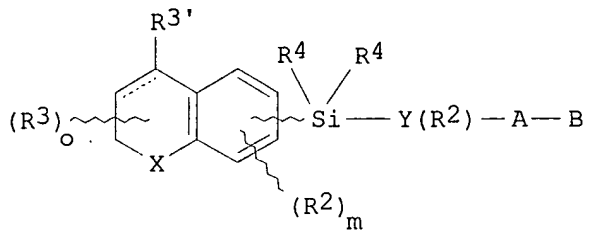
IT Alkadienes
RL: IMF (Industrial manufacture); PREP (Preparation)
(1,4-; prepn. of 1,4-dienes with high selectivity from 1,3-diens and ethylene)
IT 97-93-8, Triethylaluminum, uses 121-44-8, Triethylamine, uses
607-01-2, Diphenylphosphinoethane 14024-18-1, Iron acetylacetonate
37275-48-2, Bipyridyl
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prepn. of 1,4-dienes with high selectivity from 1,3-diens and ethylene)
IT 145414-95-5P 318269-42-0P, 1,?-Heptadiene 318269-43-1P
RL: IMF (Industrial manufacture); PREP (Preparation)
(prepn. of 1,4-dienes with high selectivity from 1,3-diens and ethylene)
IT 74-85-1, Ethylene, reactions 78-79-5, Isoprene, reactions
504-60-9, 1,3-Pentadiene 2288-18-8, 2-Phenyl-1,3-butadiene
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 1,4-dienes with high selectivity from 1,3-diens and ethylene)

L13 ANSWER 4 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 134:42260 MARPAT
TITLE: Organosilyl compounds having nuclear hormone receptor modulating activity
INVENTOR(S): Beard, Richard L.; Garst, Michael; Chandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

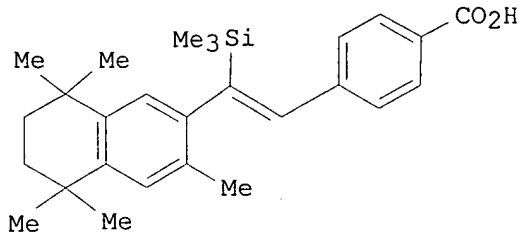
Bad date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000077011	A1	20001221	WO 2000-US15972	20000609
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1185539	A1	20020313	EP 2000-941321	20000609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000011741	A	20020319	BR 2000-11741	20000609
PRIORITY APPLN. INFO.:			US 1999-138731P	19990611
			WO 2000-US15972	20000609

GI



I



II

AB The prepn. of silicon-contg. org. compds., I (X = O, S, NR', R' = C1-6 alkyl; R2 = H, C1-6 alkyl, F, Cl, Br, I, CF3, OH, SH, C1-12 alkoxy, alkylthio, etc.; R3 = H, C1-6 alkyl, F; m = 0-3; o = 0-4; R3' = H, C1-6 alkyl, F, heteroaryl with 1-3 hetero atoms, etc.; R4 = C1-8 alkyl, Ph, etc.; Y = Ph, naphthyl, heteroaryl, etc.; A = (CH2)q, q = C3-6 alkyl, C3-6 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl, etc.; B = H, CO2H, NO2, P(O)(OH)2, etc.), useful as modulators of mammalian nuclear hormone receptors, particularly the retinoid receptors and the farnesoid receptors, is described. Thus, silylation of 4-BrC6H4CH2OH with Ph2(t-Bu)SiCl in CH2Cl2 in the presence of Et3N gave 4-BrC6H4CH2OSiPh2Bu-t which on coupling with Me3SiC.tplbond.CH gave 4-Me3SiC.tplbond.CC6H4CH2OSiPh2Bu-t. Borane mediated coupling of 4-Me3SiC.tplbond.CC6H4CH2OSiPh2Bu-t with 2-bromo-3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalene followed by MnO2 oxidn. and hydrolysis gave title compd. II.

IC ICM C07F007-08

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 1

ST organo silyl compd prepn hormone receptor modulating activity; retinoid receptor organo silyl compd prepn

IT Hormone receptors
Retinoid receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(prepn. of organosilyl compds. having nuclear hormone receptor modulating activity)

IT 27452-17-1 119999-22-3, 2-Bromo-3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalene
RL: RCT (Reactant); RACT (Reactant or reagent)
(borane mediated coupling reaction with silylethynylbenzyl silyl ether)

IT 5798-75-4, Ethyl 4-bromobenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction with (trimethylsilyl)acetylene)

IT 312738-91-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction with Et silylethynylbenzoate)
IT 312738-92-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction with bromo-tert-butylphenyldimethyldihydronaph
thalene)
IT 1066-54-2, (Trimethylsilyl)acetylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction with bromobenzyl silyl ether)
IT 22385-77-9, 1-Bromo-3,5-di-tert-butylbenzene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction with silylethynylbenzyl silyl ether)
IT 312738-30-0P 312738-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and borane mediated coupling reaction with
bromopentamethyltetrahydronaphthalene)
IT 150969-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and coupling reaction with bromotetramethylchroman)
IT 133776-42-8P 312738-59-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and coupling reaction with trimethylsilylacetylene)
IT 312738-41-3P 312738-52-6P 312738-57-1P 312738-65-1P
312738-69-5P 312738-74-2P 312738-79-7P 312738-82-2P
312738-86-6P 312738-89-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and hydrolysis of)
IT 188889-06-7P 300537-62-6P 312738-36-6P 312738-49-1P
312738-64-0P 312738-68-4P 312738-72-0P 312738-77-5P
312738-81-1P 312738-85-5P 312738-88-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and oxidn. of)
IT 312738-45-7P 312738-55-9P 312738-58-2P 312738-67-3P
312738-70-8P 312738-75-3P 312738-80-0P 312738-84-4P
312738-87-7P 312738-90-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(prepn. of organosilyl compds. having nuclear hormone receptor
modulating activity)
IT 58479-61-1, tert-Butyldiphenylsilyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation of bromobenzyl alc. with)
IT 1719-53-5, Diethyldichlorosilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation with bromotetramethyltetrahydronaphthalene)
IT 873-75-6, 4-Bromobenzyl alcohol 79387-71-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation with tert-butyldiphenylsilyl chloride)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L13 ANSWER 5 OF 18 MARPAT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 134:37038 MARPAT
TITLE: Methods for modulating FXR receptor activity
INVENTOR(S): Forman, Barry M.; Beard, Richard L.; Gyhandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc.; USA
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

Bad date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000076523	A1	20001221	WO 2000-US15912	20000609
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1185277	A1	20020313	EP 2000-941312	20000609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.:			US 1999-138731P	19990611
			WO 2000-US15912	20000609

AB Methods for modulating the activity of the mammalian FXR (farnesoid X-activated receptor). The methods include methods of treating a hyper- or hypocholesterolemic mammal comprising contacting the mammal with synthetic compds. having FXR receptor activity.

IC A61K031-695; A61P035-00; A61P009-10
CC 1-10 (Pharmacology)
Section cross-reference(s): 29
ST FXR receptor modulation hypercholesterolemia treatment; hypocholesterolemia treatment FXR receptor modulation; farnesoid X receptor modulation hypocholesterolemia treatment
IT Nuclear receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(FXR (farnesoid X-activated receptor); methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)
IT Anticholesteremic agents
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)
IT Retinoid X receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)
IT Bile acids
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation,

nonpreparative); PROC (Process)
(modulation of prodn. of; methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

IT 57-88-5, Cholesterol, biological studies
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(blood, hypocholesterolemia, treatment of; methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

IT 312738-36-6P 312738-41-3P 312738-49-1P 312738-52-6P
312738-57-1P 312738-64-0P 312738-65-1P 312738-68-4P
312738-69-5P 312738-72-0P 312738-74-2P 312738-77-5P
312738-79-7P 312738-81-1P 312738-82-2P 312738-85-5P
312738-86-6P 312738-88-8P 313219-43-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

IT 312738-45-7P 312738-55-9P 312738-58-2P 312738-67-3P
312738-70-8P 312738-75-3P 312738-80-0P 312738-84-4P
312738-87-7P 313219-44-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

IT 71441-28-6, TTNPB 313268-94-9, AGN 10
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

IT 873-75-6, 4-Bromobenzyl alcohol 1066-54-2, (Trimethylsilyl)acetylene 5798-75-4, Ethyl 4-bromobenzoate 22385-77-9, 1-Bromo-3,5-di-tert-butylbenzene 27452-17-1 58479-61-1, tert-Butyldiphenylsilyl chloride 79387-71-6 119999-22-3, 2-Bromo-3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalene 188889-06-7 201142-10-1 300537-62-6 312738-91-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in relation to role of RXR receptor)

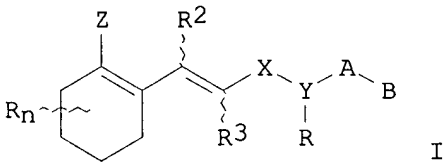
IT 133776-42-8P, 4-Bromobenzyl tert-butyldiphenylsilyl ether 150969-54-3P 312738-30-0P 312738-59-3P 312738-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methods for modulating FXR (farnesoid X-activated) receptor activity and treatment of hyper- and hypocholesterolemia in

relation to role of RXR receptor)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 133:349995 MARPAT
TITLE: Preparation of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compounds and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biological activity
INVENTOR(S): Beard, Richard L.; Colon, Diana F.; Chandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068190	A2	20001116	WO 2000-US11975	20000503
WO 2000068190	A3	20010118		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6177588	B1	20010123	US 1999-307073	19990507
PRIORITY APPLN. INFO.:			US 1999-307073	19990507

GI



I

AB The title compds. I [R1 = alkyl, Ph, heteroaryl, RCO, RCS, trifluoromethylsulfonyl, trialkylsilyl; Z = W1R1 or W2; W1 = O, S; W2 = CH2OR2, R2CO, CN, etc.; R = H, lower alkyl of 1 to 10 carbons, cycloalkyl of 3 to 10 carbons, halo, etc.; R2, R3 = lower alkyl of 1 to 10 carbons, cycloalkyl; n = 0-6; X = C.tplbond.C, CO2, etc.; Y = Ph, naphthyl, heteroaryl; A = (CH2)q; B = H, CO2H, etc.], having retinoid antagonist or retinoid neg. hormone like biol. activity, were prepd. E.g., Et (E)-4-(4-(2,2-dimethyl-6-(trifluromethanesulfonyl)oxycyclohex-1-enyl)but-3-en-1-ynyl)benzoate was prepd.

IC ICM C07C403-00
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 1
ST cyclohexene alkoxy acyloxy prepn retinoid like activity
IT Retinoids
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(prepn. of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compds. and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biol. activity)
IT 208253-12-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compds. and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biol. activity)
IT 208253-13-8P 305818-72-8P 305818-73-9P 305818-74-0P 305818-75-1P 305818-76-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compds. and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biol. activity)
IT 51934-41-9, Ethyl 4-iodobenzoate 305818-77-3 305818-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compds. and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biol. activity)
IT 10602-03-6P, Ethyl 4-ethynylbenzoate 208253-10-5P 208253-11-6P 305818-79-5P 305818-80-8P 305818-81-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 1-alkoxy and 1-acyloxy substituted cyclohex-1-ene compds. and sulfur and 1-alkoxycarbonyl analogs having retinoid-like biol. activity)

L13 ANSWER 7 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 133:238475 MARPAT
TITLE: Hydrolyzable and polymerizable silanes, their preparation and use
INVENTOR(S): Wolter, Herbert; Schmitzer, Siegfried
PATENT ASSIGNEE(S): Fraunhofer-Gesellschaft zur Forderung der Angewandten Forschung e.V., Germany
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000053612	A1	20000914	WO 2000-DE765	20000307

W: AU, BR, CA, CZ, KR, NO, NZ, PL, SI, TR, US, AM, AZ, BY, KG,

Bad date

KZ, MD, RU, TJ, TM
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
DE 19910895 A1 20000921 DE 1999-19910895 19990311
EP 1159281 A1 20011205 EP 2000-916815 20000307
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE, PT, SI, FI
PRIORITY APPLN. INFO.: DE 1999-19910895 19990311
WO 2000-DE765 20000307

AB The silanes have the formula {[B(CONHR1]eR0c}bSiXaR4-a-b)d, where B is a C2-50 org. residue with .gtoreq.1 C-C double bond, R = (un)substituted C1-15 alkyl, alkenyl, aryl, alkylaryl or arylalkyl, R0 and R1 = (un)substituted alkylene, alkenylene, arylene, alkylenearylene or arylenealkylene, X = H, halogen, OH, alkoxy, acyl, acyloxy, alkoxycarbonyl or NR22, R2 = H, alkyl or aryl, a and b = 1-3, a + b = 2-4, c = 0 or 1, d = 1-10, and e = 1-4, and are used in the prodn. of silicic acid (hetero)polycondensates and (hetero)polymers. Thus, glycerol 1,3-dimethacrylate was esterified with succinic anhydride, and the product was treated with (EtO)3Si(CH2)3NCO to give (CH2:CMeCO2CH2)2CHO2CCH2CH2CONH(CH2)3Si(OEt)3, which was hydrolyzable to form a coating material that could be cured by radical polymn. of the methacrylate groups or their copolymn. with dodecamethylene dimethacrylate. The copolymer was also useful in dental fillings or prostheses.

IC ICM C07F007-12
ICS C07F007-18; C07F007-10; C08G077-20; C08G077-22; C08F030-08

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 42, 63

ST unsatd hydrolyzable silane monomer; dental composite unsatd hydrolyzable silane

IT Dental materials and appliances
(composites; prepn. of hydrolyzable and polymerizable silanes for use in)

IT Adhesives
Coating materials
Contact lenses
Sealing compositions
(prepn. of hydrolyzable and polymerizable silanes for use in)

IT 293727-39-6P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(prepn. of hydrolyzable and polymerizable silanes)

IT 293727-40-9P 293727-41-0P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(prepn. of hydrolyzable and polymerizable silanes)

IT 24801-88-5 293727-38-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of hydrolyzable and polymerizable silanes)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 132:166736 MARPAT
TITLE: Mixture of fluoroarylaluminum and aryloxyaluminum catalyst activator composition for olefin polymerization
INVENTOR(S): Chen, Eugene Y.; Kruper, William J., Jr.; Roof,

Gordon R.; Schwartz, David J.; Storer, Joey W.
PATENT ASSIGNEE(S): The Dow Chemical Co., USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4

Bad date

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009514	A1	20000224	WO 1999-US13345	19990611
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9945646	A1	20000306	AU 1999-45646	19990611
US 6211111	B1	20010403	US 1999-330675	19990611
EP 1105398	A1	20010613	EP 1999-928617	19990611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 2001018396	A1	20010830	US 2001-772592	20010130
US 6387838	B2	20020514		
PRIORITY APPLN. INFO.:			US 1998-96800P	19980817
			US 1998-100490P	19980916
			US 1999-330675	19990611
			WO 1999-US13345	19990611

AB The activators are described as aryloxyaluminum compds. AlArfQ1Q2, or a dimer, adduct, or mixt. that are mixed with Al compds. AlArf3 at ratio 1:0.1-10, where Arf is a fluorinated arom. hydrocarbonyl moiety of 6-30 C atoms; Q1 = Arf or a C1-20 hydrocarbyl group, optionally substituted with .gtoreq.1 cyclohydrocarbyl, hydrocarbyloxy, hydrocarbylsiloxy, hydrocarbylsilylamino, hydrocarbylsilyl, silylhydrocarbyl, di(hydrocarbylsilyl)amino, hydrocarbylamino, di(hydrocarbyl)amino, di(hydrocarbyl)phosphino, or hydrocarbylsulfido groups having 1-20 atoms other than H, or further optionally, such substituents may be covalently linked with each other to form .gtoreq.1 fused rings or ring systems; and Q2 = aryloxy, arylsulfide or di(hydrocarbyl)amido group, optionally substituted with .gtoreq.1 hydrocarbyl, cyclohydrocarbyl, hydrocarbyloxy, hydrocarbylsiloxy, hydrocarbylsilylamino, hydrocarbylsilyl, silylhydrocarbyl, di(hydrocarbylsilyl)amino, hydrocarbylamino, di(hydrocarbyl)amino, di(hydrocarbyl)phosphino, or hydrocarbylsulfido groups having 1-20 atoms other than H, or, further optionally such substituents may be covalently linked with each other to form .gtoreq.1 fused rings or ring systems, the Q2 having 3-20 atoms other than H. An example activator was a mixt. of tris(perfluorophenyl)aluminum and diisobutyl-(2,6-tert-butyl-4-methylphenoxy)aluminum.

IC ICM C07F005-06
ICS C08F010-00

CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67

ST aryloxyaluminum polymn catalyst activator; titanium metallocene polymn catalyst olefin; trisperfluorophenyl aluminum mixt aryloxyaluminum activator

IT Polymerization catalysts
(activators; metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

IT 255884-99-2P 258883-20-4P 259141-07-6P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(activators; metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

IT 56252-56-3, Diisobutyl-(2,6-di-tert-butyl-4-methylphenoxy)aluminum 168704-96-9
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(activators; metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

IT 169104-71-6
RL: CAT (Catalyst use); USES (Uses)
(metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

IT 25085-53-4P, Isotactic polypropylene 26221-73-8P, Ethylene-1-octene copolymer
RL: IMF (Industrial manufacture); PREP (Preparation)
(metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

IT 130139-66-1 135072-62-7 197641-03-5 203068-22-8 210301-31-8 223645-35-0 240136-02-1 240136-04-3
RL: CAT (Catalyst use); USES (Uses)
(metallocene; metallocene and aryloxyaluminum catalyst activator mixt. for olefin polymn.)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 131:102289 MARPAT
TITLE: Preparation of xanthine derivatives as P-450 inhibitors
INVENTOR(S): Klein, J. Peter; Kumar, Anil M.; Woodson, Paul
PATENT ASSIGNEE(S): Cell Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Bad date ✓

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9935148	A1	19990715	WO 1999-US34	19990104

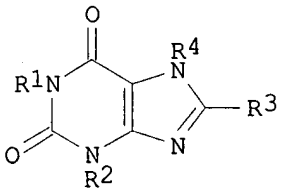
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6075029	A	20000613	US 1998-2345	19980102
AU 9919508	A1	19990726	AU 1999-19508	19990104
PRIORITY APPLN. INFO.:			US 1998-2345	19980102
			WO 1999-US34	19990104

GI



I

AB Xanthine compds. I (R1 = .omega.-1 secondary alc.-substituted alkyl; R2 = alkyl, alkenyl, alkynyl; R3 = CH2Y and Y = alkyl, alkenyl, alkynyl; R4 = H, CH2Y) were prepd. I are useful in affecting drug metab. and, particularly, in extending the circulating half-life of compds. that are metabolized via P 450-mediated pathways. E.g., (R)-1-(5-hydroxyhexyl)-3,8-dimethylxanthine was prepd.

IC C07D473-04; A61K031-52

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST xanthine prepn P 450 inhibitor

IT 230644-80-1P 230644-81-2P 230954-82-2P, CT 2408R 230954-83-3P, CT 2408S 230954-84-4P, CT 2412R 230954-86-6P, CT 2412S
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of xanthine derivs. as P 450 inhibitors)

IT 9035-51-2, P 450, biological studies
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(prepn. of xanthine derivs. as P 450 inhibitors)

IT 100-39-0, Benzyl bromide 617-89-0, Furfurylamine 2434-53-9, 6-Amino-1-methyluracil 18997-19-8, Chloromethyl pivalate 154885-34-4 230644-82-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of xanthine derivs. as P 450 inhibitors)

IT 5962-13-0P, Furfurylurea 6972-82-3P, 5,6-Diamino-1-methyluracil 82448-39-3P, 3,8-Dimethylxanthine 131598-98-6P 230644-83-4P 230644-84-5P 230644-85-6P 230644-86-7P 230644-87-8P 230644-88-9P 230644-89-0P 230644-90-3P 230644-91-4P 230644-92-5P 230644-93-6P 230644-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of xanthine derivs. as P 450 inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 130:168477 MARPAT

TITLE: Preparation of 2-silylalkenylboranes
INVENTOR(S): Onosawa, Shunya; Hatanaka, Yasuo; Tanaka, Masato
PATENT ASSIGNEE(S): Agency of Industrial Sciences and Technology, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11012285	A2	19990119	JP 1997-162175	19970619
JP 2963985	B2	19991018		

OTHER SOURCE(S): CASREACT 130:168477

AB R1R2R3SiCR6:CR7BR4R5 (I; R1-R3 = aliph. or arom. group; R4, R5 = halo, alkoxy, aryloxy, amino; R4R5 may form ring; R6, R7 = H, aliph. or arom. group, silyl) are prepd. by reaction of R1R2R3SiBR4R5 (R1-R5 = same as I) with R6C.tplbond.CR7 (R6, R7 = same as I) in the presence of catalysts comprising Group 10 metals, their complexes, or their salts. 1-Octyne was reacted with 1,3-dimethyl-2-(dimethylphenylsilyl)-1,3-diaza-2-boracyclopentane in C6H6 in the presence of tris(dibenzylideneacetone)dipalladium and 4-ethyl-1-phospha-2,6,7-trioxabicyclo[2.2.2]octane at 80.degree. for 2 h to give 92% (Z)-I (R1 = R2 = Me, R3 = Ph, R4R5 = NMeCH2CH2NMe, R6 = n-hexyl, R7 = H).

IC ICM C07F007-08
ICS B01J031-24; C07F007-10; C07B061-00

CC 29-6 (Organometallic and Organometalloidal Compounds)

ST silylalkenylborane prepn; borane silyl alkenyl prepn; alkyne addn silylborane Group 10 catalyst

IT Group VIII element compounds
RL: CAT (Catalyst use); USES (Uses)
(Group 10, salts; catalysts in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using)

IT Group VIII element complexes
Group VIII elements
RL: CAT (Catalyst use); USES (Uses)
(Group 10; catalysts in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using)

IT Addition reaction catalysts
(prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)

IT 14221-01-3, Tetrakis(triphenylphosphine)palladium 51364-51-3, Tris(dibenzylideneacetone)dipalladium
RL: CAT (Catalyst use); USES (Uses)
(catalyst in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)

IT 594-09-2, Trimethylphosphine 824-11-3, 4-Ethyl-1-phospha-2,6,7-trioxabicyclo[2.2.2]octane
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)

IT 193903-46-7P 193903-47-8P 193903-49-0P 193903-51-4P
220368-08-1P 220368-09-2P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)
IT 2396-63-6, 1,6-Heptadiyne
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)
IT 536-74-3, Ethynylbenzene 629-05-0, 1-Octyne 871-84-1, 1,7-Octadiyne 193903-45-6, 1,3-Dimethyl-2-(dimethylphenylsilyl)-1,3-diaza-2-boracyclopentane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in prepn. of silylalkenylboranes by addn. reaction of silylboranes to alkynes using Group 10 catalysts)

L13 ANSWER 11 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 130:95697 MARPAT
TITLE: Synthesis and use of retinoid compounds having negative hormone and/or antagonist activities
INVENTOR(S): Klein, Elliott S.; Johnson, Alan T.; Standeven, Andrew M.; Beard, Richard L.; Gillett, Samuel J.; Duong, Tien T.; Nagpal, Sunil; Vuligonda, Vidyasagar; Teng, Min; Chandraratna, Roshantha A.
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 252 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

wrong Compd

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9858922	A1	19981230	WO 1998-US13065	19980624
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5877207	A	19990302	US 1997-880823	19970624
AU 9882619	A1	19990104	AU 1998-82619	19980624
AU 729140	B2	20010125		
EP 991636	A1	20000412	EP 1998-932821	19980624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9810340	A	20000919	BR 1998-10340	19980624
JP 2002507204	T2	20020305	JP 1999-504998	19980624
PRIORITY APPLN. INFO.:			US 1997-880823	19970624
			US 1996-613863	19960311
			WO 1998-US13065	19980624

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Retinoid analogs I [A = (R3)o; B = (R15)r; C = (F)s; X = C(R1)2, O; R1 = H, C1-6-alkyl; R2 = C1-6-alkyl, F, Cl, Br, I, CF3, C1-6-fluoroalkyl, OH, SH, C1-6-alkoxy, C1-6-alkylthio; m, o = 0 - 3; R3 = F, C1-6-alkyl; s = 1 - 3; R8 = C1-10-alkyl, trimethylsilylalkyl, C5-10-cycloalkyl, Ph, alkylphenyl; R15 = H, F, Cl, Br, I, NO2, N(R8)2, COR8, NR8CON(R8)2, O2CR8, OR8, CN, C1-10-alkyl, C1-10-alkenyl, C1-10-alkadienyl, C1-10-alkatrienyl, C1-10-alkynyl, C1-10-alkadiynyl, C1-10-alkatriynyl, trialkylsilyl, trialkylsilyloxy; r = 0 - 5; CONH at C(6) or C(7) of benzopyran ring or C(2) or C(3) of dihydronaphthalene ring] having neg. hormone and/or antagonist activities are described. Thus, retinoid analog II was prepd. from dihydrocoumarin via condensation of benzopyrancarboxylate III with p-tolylmagnesium bromide and amidation of tolylbenzopyrancarboxylic acid IV with Et 4-amino-2,6-difluorobenzoate. In the ligand binding assay II showed Kd = 0.69 nm for receptor RAR.alpha., Kd = 541 nm for receptor RAR.beta. and Kd = 7280 nm for receptor RAR.gamma..

IC ICM C07D311-58
ICS C07C233-81; C07F007-18; A61K031-215; A61K031-335

CC 30-20 (Terpenes and Terpenoids)
Section cross-reference(s): 1, 2, 63

ST retinoid analog prepn neg hormone receptor antagonist

IT Retinoic acid receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(RAR-.alpha.; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT Retinoic acid receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(RAR-.beta.; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT Retinoic acid receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(RAR-.gamma.; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT Retinoids
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(analogs; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT Steroids, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(hormones; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT Hormones, animal, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(steroid; synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT 166977-56-6P 171746-21-7P 180920-66-5P 182560-49-2P
182560-50-5P 188888-00-8P 188888-02-0P 188888-04-2P
188888-06-4P 188888-08-6P 188888-11-1P 188888-14-4P
188888-16-6P 188888-18-8P 188888-20-2P 188888-22-4P
188888-24-6P 188888-26-8P 188888-30-4P 188888-43-9P
188888-47-3P 188888-55-3P 188888-67-7P 188888-80-4P
188888-84-8P 188888-88-2P 192817-12-2P 219320-77-1P
219320-78-2P 219320-79-3P 219320-80-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT 94-09-7, Ethyl 4-aminobenzoate 95-46-5, o-Bromotoluene 104-92-7, 1-Bromo-4-methoxybenzene 106-38-7, 4-Bromotoluene 106-39-8, 1-Bromo-4-chlorobenzene 106-53-6, 4-Bromothiophenol 109-04-6, 2-Bromopyridine 110-00-9, Furan 110-02-1, Thiophene 119-84-6 120-47-8, Ethyl 4-hydroxybenzoate 288-47-1, Thiazole 402-43-7, 1-Bromo-4-(trifluoromethyl)benzene 554-14-3, 2-Methylthiophene 556-96-7, 1-Bromo-3,5-dimethylbenzene 580-13-2, 2-Bromonaphthalene 590-92-1, 3-Bromopropionic acid 591-17-3 619-58-9, 4-Iodobenzoic acid 619-66-9, 4-Formylbenzoic acid 626-55-1, 3-Bromopyridine 637-59-2, 1-Bromo-3-phenylpropane 693-95-8, 4-Methylthiazole 1585-07-5, 4-Ethylbromobenzene 2537-48-6, Diethyl (cyanomethyl)phosphonate 2715-43-7, Ethyl 4-vinylbenzoate 3430-13-5, 5-Bromo-2-methylpyridine 3581-89-3, 5-Methylthiazole 3581-91-7, 4,5-Dimethylthiazole 3972-65-4, 1-Bromo-4-(tert-butyl)benzene 4294-57-9, 4-Tolylmagnesium bromide 5326-23-8, 6-Chloronicotinic acid 7476-79-1, Ethyl 4-nitrosobenzoate 39760-56-0 65423-56-5, 1-Bromo-3-[(tert-butyldimethylsilyl)oxy]benzene 67159-84-6 67963-68-2, 1-Bromo-4-[(tert-butyldimethylsilyl)oxy]benzene 73792-06-0, Ethyl 4-amino-2-fluorobenzoate 176700-52-0 191469-36-0, Ethyl 4-amino-2,6-difluorobenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT 1198-96-5P, 2,2-Dimethylchroman 1590-25-6P 1985-59-7P, 1,1-Dimethyltetralin 2039-47-6P, 2,2-Dimethylchroman-6-carboxylic acid 2979-69-3P, 3,4-Dihydro-4,4-dimethyl-1(2H)-naphthalenone 2979-70-6P 5773-80-8P 6630-24-6P 13054-02-9P, 6-Iodonicotinic acid 13735-04-1P 13735-13-2P 32333-31-6P 33209-71-1P 51934-41-9P, Ethyl 4-iodobenzoate 86471-14-9P 150932-04-0P 151917-39-4P, Ethyl 6-iodonicotinate 166977-92-0P 166977-93-1P 166978-45-6P 166978-46-7P, 7-Bromo-3,4-dihydro-4,4-dimethyl-1(2H)-naphthalenone 166978-48-9P 166978-49-0P 171568-43-7P
171568-44-8P 180920-20-1P 180920-21-2P 180920-22-3P
180920-64-3P 180920-65-4P 188887-70-9P 188887-72-1P
188887-74-3P 188887-76-5P 188887-79-8P 188887-81-2P
188887-83-4P 188887-86-7P 188887-88-9P 188887-94-7P
188887-96-9P 188887-98-1P 188888-28-0P 188888-33-7P
188888-41-7P 188888-45-1P 188888-49-5P 188888-53-1P
188888-57-5P 188888-61-1P 188888-65-5P 188888-78-0P
188888-86-0P 188888-90-6P 188889-20-5P 188889-22-7P
188889-23-8P 188889-25-0P 188889-27-2P 188889-29-4P

188889-33-0P 188889-35-2P 188889-37-4P 188889-39-6P
188889-41-0P 188889-45-4P 188889-47-6P 188889-49-8P
188889-51-2P 188889-53-4P 188889-55-6P 188889-57-8P
188889-60-3P 188889-63-6P 188889-66-9P 192762-68-8P
192762-69-9P 192762-70-2P 192762-71-3P 192762-72-4P
192762-73-5P 192762-74-6P 219320-73-7P 219320-74-8P
219320-75-9P 219320-76-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT 150932-00-6P 180920-67-6P 188887-90-3P 188887-92-5P
188888-39-3P 188888-51-9P 188888-59-7P 188888-63-3P
188888-92-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

IT 166977-57-7P 180920-30-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and use of retinoid compds. having neg. hormone and/or antagonist activities)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 129:82073 MARPAT
TITLE: Metal bisenolate complex catalysts for the production of functionalized polymers
INVENTOR(S): Erker, Gerhard; Spather, Wolf; Fritze, Cornelia; Mecking, Stefan
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 848015	A1	19980617	EP 1997-121287	19971204
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
DE 19651442	A1	19980618	DE 1996-19651442	19961211
JP 10182713	A2	19980707	JP 1997-341072	19971211
CN 1187492	A	19980715	CN 1997-120872	19971211
BR 9705524	A	19990629	BR 1997-5524	19971211
PRIORITY APPLN. INFO.:			DE 1996-19651442	19961211

AB Catalysts for the manuf. of polymers contg. functional groups contain at least one metal bis(enolate) in which both enolate groups are bonded to the metal by a covalent single bond and at least one cocatalyst. Thus, lithium propen-2-olate and biscyclopentadienylzirconium dichloride were reacted in THF to give orange-red biscyclopentadienylzirconium bis(propen-2-olate) (I). Polymn. of Me vinyl ketone in methylene chloride contg. I and tris(pentafluorophenyl)borane yielded an amber-colored polymer.

IC ICM C08F004-60
ICS C07F017-00
CC 35-3 (Chemistry of Synthetic High Polymers)
ST dicyclopentadienyl metal bispropenolate polymn catalyst; zirconium bisenolate complex polymn catalyst; hafnium bisenolate complex polymn catalyst; titanium bisenolate complex polymn catalyst; vinyl compd polymn catalyst
IT Polymerization catalysts
(prepn. of catalysts for manuf. of polymers contg. functional groups)
IT 209158-19-0P 209158-20-3P 209158-21-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalyst; prepn. of catalysts for manuf. of polymers contg. functional groups)
IT 1109-15-5, Tris(pentafluorophenyl)borane
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst, contg. metal bisenolate complex; for manuf. of polymers contg. functional groups)
IT 1109-15-5DP, Tris(pentafluorophenyl)borane, reaction products with biscyclopentadienylzirconium bis(propen-2-olate) 25038-87-3P, Methyl vinyl ketone homopolymer 209158-20-3DP, reaction products with tris(pentafluorophenyl)borane
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of catalysts for manuf. of polymers contg. functional groups)
IT 1271-19-8, Biscyclopentadienyltitanium dichloride 1291-32-3, Biscyclopentadienylzirconium dichloride 12116-66-4, Biscyclopentadienylhafnium dichloride 67863-40-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; in prepn. of catalysts for manuf. of polymers contg. functional groups)

L13 ANSWER 13 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 129:54376 MARPAT
TITLE: Preparation of 3H-1,2,4-triazol-3-one derivatives as fungicides and arthropodicides
INVENTOR(S): Brown, Richard James; Castro, Peter Paul; Chan, Dominic Ming-Tak; Daub, John Powell; Koether, Gerard Michael; Selby, Thomas Paul; et al.
PATENT ASSIGNEE(S): E.I. Du Pont De Nemours and Company, USA; Brown, Richard James; Castro, Peter Paul; Chan, Dominic Ming-Tak; Daub, John Powell; Koether, Gerard Michael
SOURCE: PCT Int. Appl., 171 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

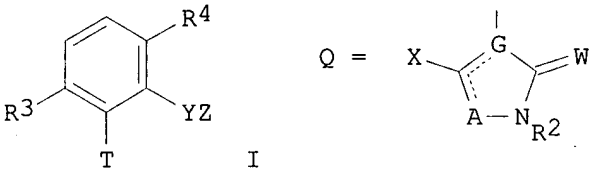
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9823156	A1	19980604	WO 1997-US21944	19971125

W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ,

TM
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

WO 9823155		A1	19980604	WO 1996-US18916	19961126
	W: JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9854633		A1	19980622	AU 1998-54633	19971125
EP 944314		A1	19990929	EP 1997-948597	19971125
	R: CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
BR 9713415		A	20000418	BR 1997-13415	19971125
JP 2001506984		T2	20010529	JP 1998-524889	19971125
PRIORITY APPLN. INFO.:				WO 1996-US18916	19961126
				US 1996-33614P	19961219
				US 1997-48844P	19970606
				WO 1997-US21944	19971125

GI



I

AB I [T = Q (X = OR1, SOmR1, halo; A = S, O, N, NR5, CF7; G = C, N; W = O, S, NH, etc.), R1OsCH:CMeCO2R5; R1ON:CMeCO2R5; etc.; R3 and R4 are each independently H or CH3, provided that R3 and R4 are not both H; Y = O, CH2O, a direct bond, etc.; Z = C1-10 alkyl or haloalkyl, (un)substituted Ph, arom. heterocyclyl, etc.], useful for controlling plant diseases caused by fungal plant pathogens or for controlling arthropods, were prepd. E.g., 4-[2-[(5-bromo-2-thienyl)oxy]-6-methylphenyl]-2,4-dihydro-5-methoxy-2-methyl-3H-1,2,4-triazol-3-one was prepd. in several steps.

IC ICM A01N043-653
ICS A01N043-00; A01N037-00; C07D249-12; C07D401-12; C07D409-12; C07D403-12; C07D405-12; C07D417-12; C07D261-12; C07D285-08; C07D277-34; C07D239-52

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 10

ST triazolone prepn fungicide arthropodicide

IT Acaricides
Fungicides
Insecticides
(prepn. of 3H-1,2,4-triazol-3-one derivs. as fungicides and arthropodicides)

IT 185686-21-9P 208513-69-3P 208513-70-6P 208513-71-7P
208513-72-8P 208513-73-9P 208513-74-0P 208513-75-1P
208513-76-2P 208513-77-3P 208513-78-4P 208513-79-5P
208513-80-8P 208513-81-9P 208513-82-0P 208513-83-1P
208513-84-2P 208513-85-3P 208513-86-4P 208513-87-5P
208513-88-6P 208513-89-7P 208513-90-0P 208513-91-1P
208513-92-2P 208513-93-3P 208513-94-4P 208513-95-5P

208513-96-6P 208513-97-7P 208513-98-8P 208513-99-9P
208514-00-5P 208514-01-6P 208514-02-7P 208514-03-8P
208514-04-9P 208514-05-0P 208514-06-1P 208514-07-2P
208514-08-3P 208514-09-4P 208514-10-7P 208514-11-8P
208514-12-9P 208514-13-0P 208514-14-1P 208514-15-2P
208514-16-3P 208514-17-4P 208514-18-5P 208514-19-6P
208514-20-9P 208514-21-0P 208514-22-1P 208514-23-2P
208514-24-3P 208514-25-4P 208514-26-5P 208514-27-6P
208514-28-7P 208514-29-8P 208514-30-1P 208514-31-2P
208514-32-3P 208514-33-4P 208514-34-5P 208514-35-6P
208514-36-7P 208514-37-8P 208514-38-9P 208514-39-0P
208514-40-3P 208514-41-4P 208514-42-5P 208514-43-6P
208514-44-7P 208514-45-8P 208514-46-9P 208514-47-0P
208514-48-1P 208514-49-2P 208514-50-5P 208514-51-6P
208514-52-7P 208514-53-8P 208514-54-9P 208514-55-0P
208514-56-1P 208514-57-2P 208514-58-3P 208514-59-4P
208514-60-7P 208514-61-8P 208514-62-9P 208514-63-0P
208514-64-1P 208514-65-2P 208514-66-3P 208514-67-4P
208514-68-5P 208514-69-6P 208514-70-9P 208514-71-0P
208514-72-1P 208514-73-2P 208514-74-3P 208514-75-4P
208514-76-5P 208514-77-6P 208514-78-7P 208514-79-8P
208514-80-1P 208514-81-2P 208514-82-3P 208514-83-4P
208514-84-5P 208514-85-6P 208514-86-7P 208514-87-8P
208515-32-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3H-1,2,4-triazol-3-one derivs. as fungicides and arthropodicides)

IT 407-14-7 620-13-3, .alpha.-Bromo-m-xylene 5330-98-3
50868-73-0, 2-Methoxy-6-methylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 3H-1,2,4-triazol-3-one derivs. as fungicides and arthropodicides)

IT 186586-75-4P 186981-90-8P 203054-49-3P 203054-50-6P
203054-51-7P 208514-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 3H-1,2,4-triazol-3-one derivs. as fungicides and arthropodicides)

L13 ANSWER 14 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 128:154513 MARPAT
TITLE: Method for stereoselective preparation of chiral metallocenes
INVENTOR(S): Schottenberger, Herwig; Denifl, Peter; Mueller, Adrian Gallus; Bildstein, Benno; Jaintner, Peter; Ernst, Eberhard; Reussner, Jens
PATENT ASSIGNEE(S): PCD Petrochemie Danubia Deutschland G.m.b.H., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19726454	A1	19980205	DE 1997-19726454	19970621
EP 816371	A1	19980107	EP 1996-110460	19960628
R: AT				

PRIORITY APPLN. INFO.: EP 1996-110460 19960628

AB Chiral metallocenes of Ti, Zr, Hf, V, Nb, Ta, or lanthanides having C-, Si-, Ge-, or Sn-contg. bridges and (substituted) cyclopentadienyl or (substituted) indenyl .pi.-bonded groups, useful as catalysts for manuf. of stereoregular polyolefins, are manufd. by reaction of alkali-metal salts of the ligands contg. the bridges with the salts of the corresponding metals as a suspension in a mixt. of arom. or aliph. (halogenated) hydrocarbons with dialkyl ethers. Thus, lithiation of 2-methyl-4-phenylindene with MeLi in Et2O, reaction of the Li salt with Me2SiCl2 in Et2O, and reaction of the resulting intermediate ZrCl4 in Et2O-hexane mixt. gave a complex with racemic isomer mixt.-meso isomer ratio 60:40 and 100:0 before and after recrystn. from CH2Cl2.

IC ICM C07F017-00
ICS C08F010-00; C08F004-642; C08F004-68
ICA C07F007-08
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67
ST chiral metallocene manuf ether hydrocarbon mixt; ethyl ether hexane solvent metallocene manuf; methylphenylindene methylsilyl zirconium complex manuf solvent; bridged chiral metallocene manuf solvent; stereoregular polyolefin manuf chiral metallocene catalyst
IT Sandwich compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(Group IVB element compds.; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Sandwich compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(Group VB element compds.; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Metallocene polymerization catalysts
(chiral; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Methyl aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Aromatic hydrocarbons, uses
Chloro hydrocarbons
Hydrocarbons, uses
RL: NUU (Other use, unclassified); USES (Uses)
(ether mixts., complexation solvent; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Solvents
(ether-hydrocarbon mixts.; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Ethers, uses
RL: NUU (Other use, unclassified); USES (Uses)
(hydrocarbon mixts., complexation solvent; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)
IT Rare earth compounds

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(metallocenes; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT Group VB element compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(sandwich compds.; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT Group IVB element compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(sandwich; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT Polyolefins
RL: IMF (Industrial manufacture); PREP (Preparation)
(stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT Chloroaromatic compounds
RL: NUU (Other use, unclassified); USES (Uses)
(stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 56423-64-4P, 2-Methylindenyllithium 187470-50-4P 202649-75-0P 202660-49-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation)
(catalyst precursor; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 75-78-5 917-54-4, Methyllithium
RL: RCT (Reactant)
(catalyst precursor; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 110-54-3, Hexane, uses
RL: NUU (Other use, unclassified); USES (Uses)
(ether mixts., complexation solvent; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 60-29-7, Ethyl ether, uses 108-20-3, Diisopropyl ether
RL: NUU (Other use, unclassified); USES (Uses)
(hydrocarbon mixts., complexation solvent; stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 153882-67-8P 187470-47-9P 202660-50-2P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

IT 9003-07-0P, Polypropylene
RL: IMF (Industrial manufacture); PREP (Preparation)
(stereoselective prepn. of chiral metallocenes for olefin polymn. catalysts)

L13 ANSWER 15 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 126:104078 MARPAT
TITLE: Stereoselective synthesis of chiral amines (dolaphenine).
INVENTOR(S): Sun, Xiaoyong; Sachdeva, Yesh P.; Wilson, Donna Kaye; Gabriel, Richard L.; Ram, Siya
PATENT ASSIGNEE(S): Pharm-Eco Laboratories, Inc., USA; Sun, Xiaoyong; Sachdeva, Yesh P.; Wilson, Donna Kaye; Gabriel, Richard L.; Ram, Siya

SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9639399	A1	19961212	WO 1996-US9140	19960606
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
CA 2224121	AA	19961212	CA 1996-2224121	19960606
AU 9659879	A1	19961224	AU 1996-59879	19960606
AU 706334	B2	19990617		
EP 846107	A1	19980610	EP 1996-917228	19960606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11507059	T2	19990622	JP 1996-501531	19960606
US 5750713	A	19980512	US 1997-916721	19970818
US 6020495	A	20000201	US 1997-986834	19971208
PRIORITY APPLN. INFO.:			US 1995-467013	19950606
			WO 1996-US9140	19960606

AB R1CH(NH2)R2 (R1 = heterocyclyl; R2 = alkyl, aryl, heterocyclyl), were prepd. by (a) contacting norephedrine with BH3 complexed with an aprotic solvent to form a reducing soln. for stereoselectively reducing stereoisomers of oximes, and (b) contacting the soln. with R1C(:NOR3)R2 (R3 = alkyl, aryl; R1, R2 as above). Thus, benzyl thiazolyl ketone anti-O-methyloxime (prepn. given) was added to a soln. prepd. from (+)-norephedrine and BH3 in THF and the mixt. was stirred 16 h at room temp. and refluxed 4 h to give 60% (S)-dolaphenine.

IC ICM C07D277-28
ICS C07C209-40
CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
ST amine chiral prepn; dolaphenine chiral prepn; oxime stereoselective redn norephedrine borane
IT Amines, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(chiral, redn. of oximes with norephedrine/borane; stereoselective synthesis of chiral amines (dolaphenine))
IT Stereoselective reduction
(redn. of oximes with norephedrine/borane; stereoselective synthesis of chiral amines (dolaphenine))
IT 185986-59-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(racemic; stereoselective synthesis of chiral amines (dolaphenine))
IT 130199-65-4P, (S)-Dolaphenine
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of chiral amines (dolaphenine))
IT 144774-97-0P, (R)-Dolaphenine

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of chiral amines (dolaphenine))

IT 103-80-0, Phenylacetyl chloride 79265-30-8, 2-Trimethylsilylthiazole
RL: RCT (Reactant)
(stereoselective synthesis of chiral amines (dolaphenine))

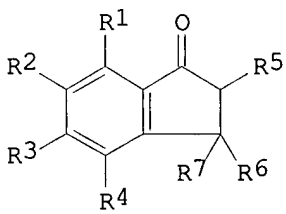
IT 144774-95-8P 144774-99-2P, Benzyl 2-thiazolyl ketone 144775-01-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of chiral amines (dolaphenine))

IT 133565-36-3P 144775-04-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of chiral amines (dolaphenine))

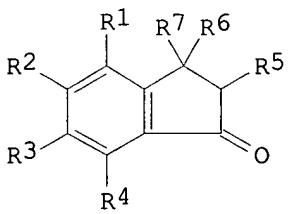
L13 ANSWER 16 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 121:35034 MARPAT
TITLE: One-step synthesis of substituted indanones
INVENTOR(S): Weisse, Laurent; Strutz, Heinz
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 587107	A1	19940316	EP 1993-114314	19930907
EP 587107	B1	19960814		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE				
AT 141250	E	19960815	AT 1993-114314	19930907
ES 2093342	T3	19961216	ES 1993-114314	19930907
FI 9303955	A	19940312	FI 1993-3955	19930909
CA 2105915	AA	19940312	CA 1993-2105915	19930910
AU 9346260	A1	19940317	AU 1993-46260	19930910
AU 667947	B2	19960418		
ZA 9306693	A	19940429	ZA 1993-6693	19930910
US 5360936	A	19941101	US 1993-120104	19930910
RU 2110510	C1	19980510	RU 1993-45021	19930910
JP 06192163	A2	19940712	JP 1993-227525	19930913
PRIORITY APPLN. INFO.:			DE 1992-4230373	19920911

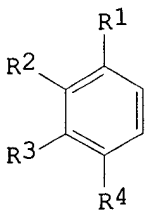
OTHER SOURCE(S): CASREACT 121:35034
GI



I



II



III

AB The title compds. (I and II; R1-R7 = H, C1-20 alkyl, C6-14 aryl, C1-10 alkoxy, C2-10 alkenyl, C7-20 arylalkyl, C6-10 haloaryl, C2-10 alkynyl, etc.) are prepd. in high yield and with a variety of substituents not readily available by prior-art synthetic processes, are prepd. by the cyclocondensation reaction of benzene III with [R6(R7)C:C(R5)CO]2O, or with the corresponding alkenoyl fluoride, in the presence of liq., anhyd. HF and BF3. Thus, biphenyl was cyclocondensed with methacrylic anhydride in the presence of HF and BF3 over 2 h at 50.degree., producing 2-methyl-5-phenylindan-1-one in 99% yield (94% selectivity).

IC ICM C07C045-46
ICS C07C049-67; C07C049-683; C07C049-697; C07C049-675

CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST methacrylic anhydride cyclocondensation biphenyl; methylphenylindanone prepn cyclocondensation biphenyl methyacrylic; indanone methylphenyl; borane fluoride cyclocondensation catalyst; hydrogen fluoride cyclocondensation catalyst

IT Cyclocondensation reaction catalysts
(boron trifluoride-hydrogen fluoride, for prepn. of substituted indanones from benzenes and methacrylic anhydrides or methacryloyl fluorides)

IT Cyclocondensation reaction
(of benzene derivs. with methacrylic anhydride derivs. or methacryloyl fluorides in presence of hydrogen fluoride and boron trifluoride)

IT 41201-58-5P 150096-51-8P 150096-57-4P 153440-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(1-step prepn. of, catalysts for)

IT 7664-39-3, Hydrogen fluoride, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts, with boron trifluoride, for cyclocondensation reaction of methacrylic anhydrides or methacryloyl fluorides with benzenes in prepn. of substituted indanones)

IT 7637-07-2, Boron trifluoride, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts, with hydrogen fluoride, for cyclocondensation of benzenes with methacrylic anhydrides or methacryloyl fluoride in prepn. of substituted indanones)

IT 91-20-3, Naphthalene, reactions 92-52-4, Biphenyl, reactions 462-06-6, Fluorobenzene
RL: RCT (Reactant)
(cyclocondensation reaction of, with methacrylic anhydride in prepn. of substituted indanones, catalysts for)

IT 760-93-0, Methacrylic anhydride
RL: RCT (Reactant)
(cyclocondensation reaction of, with naphthalin, substituted indanones from,)

L13 ANSWER 17 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 119:203149 MARPAT
TITLE: Preparation of trifluoromethyl ketones
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4201435	A1	19930722	DE 1992-4201435	19920121
WO 9314054	A1	19930722	WO 1993-EP94	19930115
W: AU, CA, HU, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9334104	A1	19930803	AU 1993-34104	19930115
AU 661560	B2	19950727		
EP 623103	A1	19941109	EP 1993-902218	19930115
EP 623103	B1	19970903		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, PT				
JP 07506337	T2	19950713	JP 1993-512154	19930115
IL 104440	A1	19980310	IL 1993-104440	19930119
HU 67802	A2	19950529	HU 1994-2140	19930121
US 5608062	A	19970304	US 1994-256523	19940921
PRIORITY APPLN. INFO.:			DE 1992-4201435	19920121
			WO 1993-EP94	19930115

OTHER SOURCE(S): CASREACT 119:203149

AB RCOCF3 [R = (substituted) aliph. hydrocarbyl, arom. hydrocrabyl] were prepd. by oxidn. of RCH(OH)CF3 by YOnH (Y = Cl, Br, iodo; n = 1-4) or salts thereof. Thus, PhCH(OH)CF3 were stirred 6 h at room temp. with 12% aq. NaOCl in CH2Cl2 contg. Bu4NHSO4 to give 75% PhCOCF3.

IC ICM C07D213-64
ICS C07D213-61; C07D213-643; C07D333-28; C07D521-00; C07D247-00; C07D277-22; C07C049-80; C07C049-84; C07C049-327

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 27

ST ketone trifluoromethyl; fluoromethyl ketone; aryltrifluoroethanol oxidn

IT Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(trifluoromethyl, prepn. of, by oxidn. of trifluoroethanols)

IT 340-04-5, 2,2,2-Trifluoro-1-phenylethanol 446-65-1 35304-69-9 67851-11-0 76911-73-4 107018-38-2 110628-69-8 128816-77-3 138624-99-4 150698-77-4 150698-78-5 150698-79-6 150698-80-9 150698-81-0 150698-82-1 150698-83-2
RL: RCT (Reactant)
(oxidn. of)

IT 394-59-2P 434-45-7P 6302-04-1P, Trifluoromethylcyclohexyl ketone 16184-89-7P 30724-22-2P 33284-21-8P, 3-Trifluoroacetylpyridine 34773-51-8P 67851-10-9P 74853-66-0P 107713-64-4P 110628-68-7P 150698-72-9P 150698-73-0P 150698-74-1P 150698-75-2P 150698-76-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by oxidn. of trifluoroethanol)

L13 ANSWER 18 OF 18 MARPAT COPYRIGHT 2002 ACS
ACCESSION NUMBER: 114:42773 MARPAT
TITLE: Preparation of dithianes as pesticides and drugs
INVENTOR(S): Casida, John Edward; Elliott, Michael; Parkin, Donald
PATENT ASSIGNEE(S): Wellcome Foundation Ltd., UK; University of California, Oakland
SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 372870	A2	19900613	EP 1989-312588	19891201
EP 372870	A3	19910116		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 02243686	A2	19900927	JP 1989-315117	19891204
PRIORITY APPLN. INFO.:			GB 1988-28326	19881205

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R1 = H, Me, Et; R2 = ethynyl, (cyano-, carboalkoxy-, HO-, halo-, etc.-substituted) hydrocarbyl, (substituted) aryl; R3, R5 = H, (substituted) Me, Et; R3R5 = bond; R4, R6 = H, (substituted) hydrocarbyl, Ph, PhCH2; R3R5 = atoms to complete a (substituted) C3-9 (bridged) ring system; not all of R3-R6 can be H, when 3 of R3-R6 = H, the other .noteq. Me; m, n = 0-2], were prepd. Thus, MeCH(SH)CH(SH)Me, 4-BrC6H4CHO, and H2CO were stirred 18 h at room temp. to give title compd. II as a mixt. of 2 isomers. Several I were active against Musca domestica, Plutella xylostella, etc., at <1000 ppm.

IC ICM C07D339-06
ICS A01N043-28

CC 28-5 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 5

ST dithiolane prepn pesticide; insecticide dithiolane; acaricide dithiolane; nematocide dithiolane; ectoaparasiticide dithiolane; drug dithiolane

IT Acaricides
Insecticides
Nematocides
Pesticides
(dithiolanes)

IT Parasiticides
(ecto-, dithiolanes)

IT 94-60-0, Dimethyl cyclohexane-1,4-dicarboxylate
RL: RCT (Reactant)
(acetylation of)

IT 4532-64-3, 2,3-Butanedithiol
RL: RCT (Reactant)
(cyclocondensation of, with bromobenzaldehyde)

IT 1122-91-4, 4-Bromobenzaldehyde 63697-96-1, 4-Ethynylbenzaldehyde
RL: RCT (Reactant)
(cyclocondensation of, with butanedithiol)

IT 23657-28-5
RL: RCT (Reactant)
(cyclocondensation of, with heptynal)

IT 534-18-9, Sodium trithiocarbonate
RL: RCT (Reactant)
(cyclocondensation of, with pentanediol dimesylate)

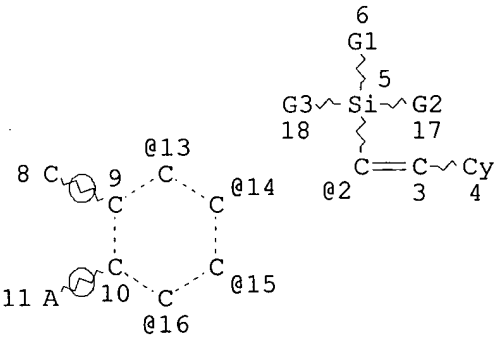
IT 130431-68-4
RL: RCT (Reactant)
(desilylation of)

IT 5343-92-0, Pentane-1,2-diol
RL: RCT (Reactant)
(mesylation of, in prepn. of dithiolane deriv.)

IT 130431-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of)
IT 130431-66-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sulfuration of)
IT 120077-74-9P 120077-75-0P, Dimethyl 1-acetylcyclohexane-1,4-dicarboxylate 120077-76-1P, Methyl 4-acetylcyclohexanecarboxylate 120077-77-2P 120077-78-3P 120077-79-4P, 4-Ethynylcyclohexylmethanol 130431-63-9P, 1,2-Pentanedithiol 130431-64-0P 130431-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for dithiolane)
IT 130431-38-8P 130431-39-9P 130431-40-2P 130431-41-3P
130431-42-4P 130431-43-5P 130431-44-6P 130431-45-7P
130431-46-8P 130431-47-9P 130431-48-0P 130431-49-1P
130431-51-5P 130431-52-6P 130431-53-7P 130431-54-8P
130431-55-9P 130431-56-0P 130431-57-1P 130431-58-2P
130431-59-3P 130431-60-6P 130431-61-7P 130431-62-8P
130462-71-4P 130462-72-5P 130462-73-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as pesticide and drug)
IT 67100-10-1, 6-Heptynal
RL: RCT (Reactant)
(reaction of, in prepn. of dithiolanes)

FILE 'MARPATPREV' ENTERED AT 11:58:59 ON 23 MAY 2002

L5 STR



VAR G1=AK/CB
VAR G2=AK/CB
VAR G3=AK/CB
VPA 2-13/14/15/16 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
MLEVEL IS CLASS ON RING NODES AND RING GROUPS

Searcher : Shears 308-4994

MLEVEL IS CLASS ON CHAIN NODES AND CHAIN GROUPS
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L14 0 SEA FILE=MARPATPREV SSS FUL L5 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 61 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

FILE 'HOME' ENTERED AT 11:59:42 ON 23 MAY 2002